



Faculty of Sciences,
Technology
and Communication



UNIVERSITÉ DU LUXEMBOURG
Research Unit in Engineering
Sciences (RUES)



Adaptive methods for multiscale fracture and surgical simulation

Stéphane Bordas & Pierre Kerfriden

University of Luxembourg and Cardiff University



Imperial College London, London, UK

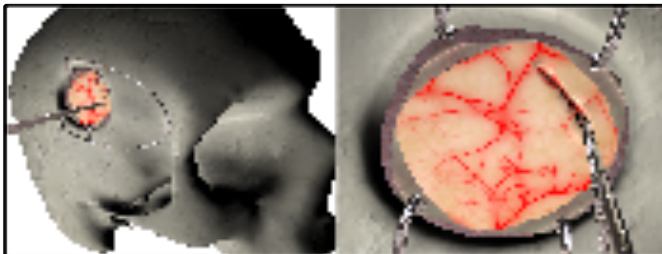
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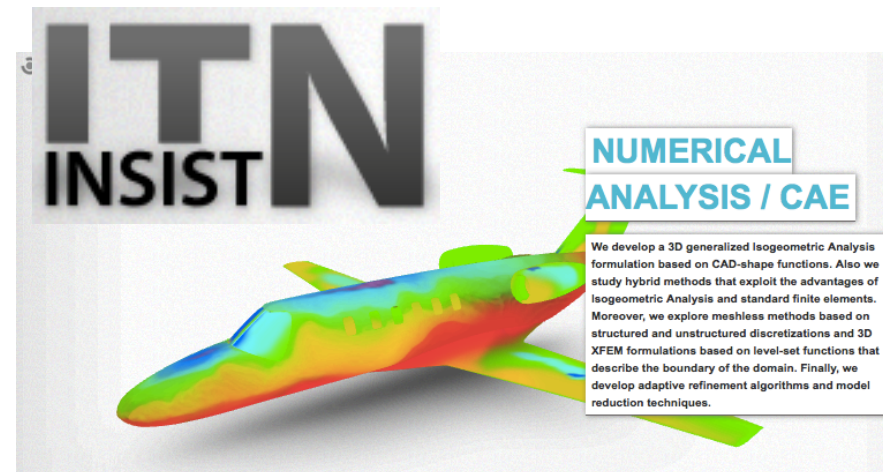
279578 - REALTCUT - Towards real time multiscale simulation of cutting in non-linear materials with applications to surgical simulation and computer guided surgery



- A small, young, dynamic university
- 3 languages (English, German, French); bilingual and trilingual degrees
- Strong mathematics and Comp. Sc.
- RUES: 3 professors in computational mechanics, 30 collaborators
- Computational sciences priority 1
- Strong local industry
- Strong and supportive national funding
- 7 EU projects in engineering, of which RealTcut: ERC Starting Grant (Bordas)



- A large, established university (1883)
- 95% 3 or 4* at RAE2008 in Civil
- Over 100 EU projects awarded of which ITN: INSIST
- Mechanics Research: 40 researchers, 14 faculty members
- Advanced manufacturing and characterisation





Advisor: Brian Moran
Now vice-provost for
faculty affairs at KAUST



1997-2003

MSc Geotechnical Engineering

PhD. Damage Tolerance of Aerospace Structures (XFEM)
and Biofilm Growth



Post-doc 2003-2006 -
Meshless/XFEM Geomechanics



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

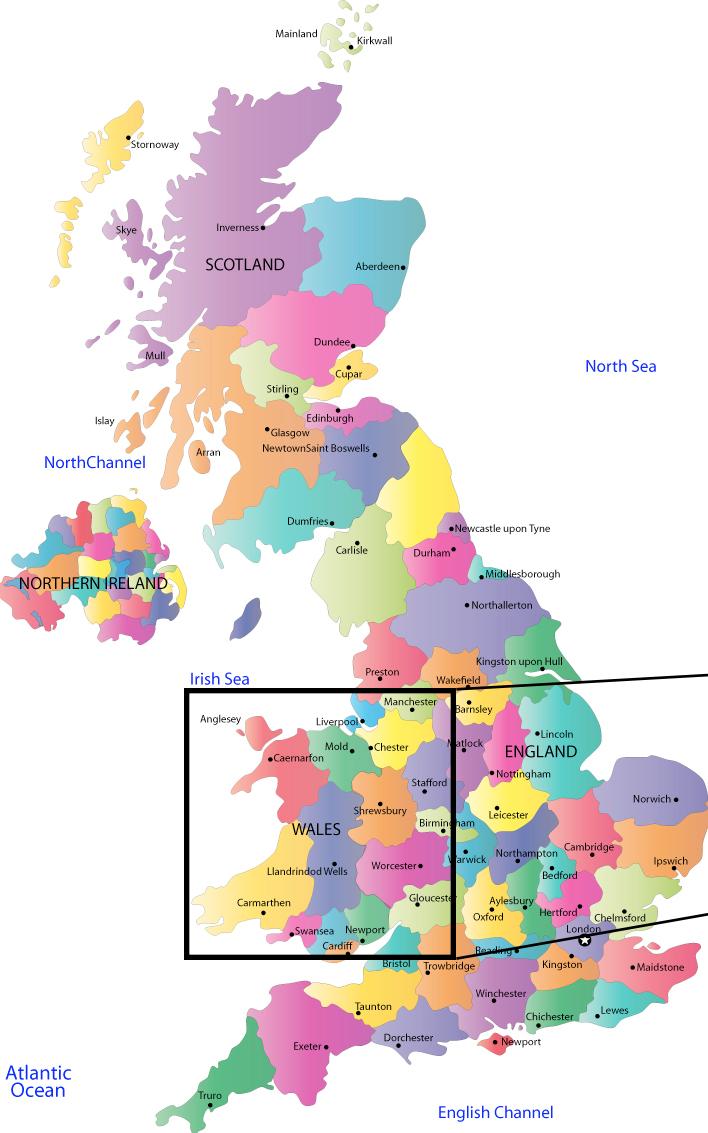




Lecturer in
civil
engineering



UNIVERSITY
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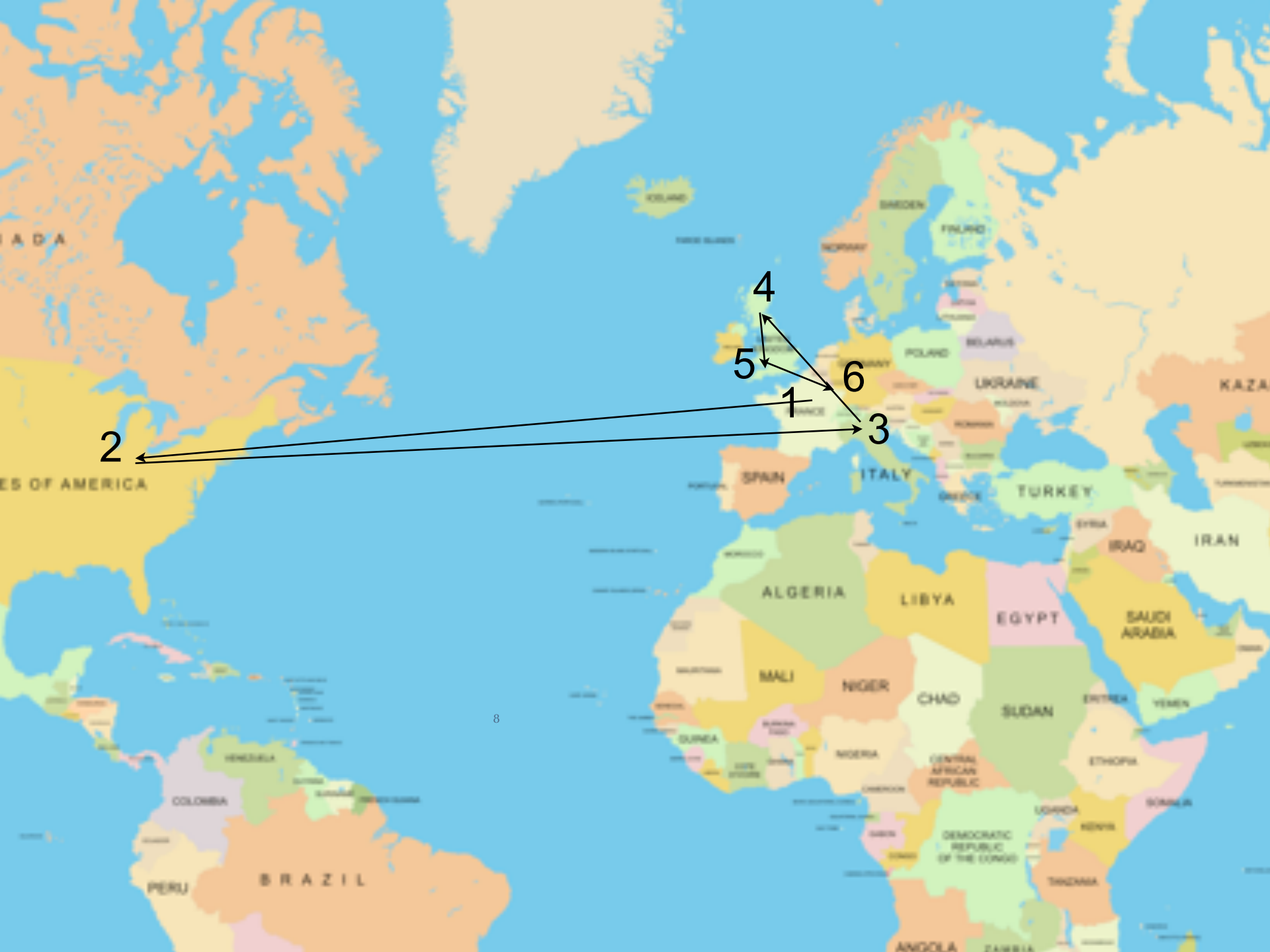
CARDIFF
UNIVERSITY

PRIFYSGOL
CAERDYDD



I M A M
Institute of Mechanics
& Advanced Materials





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Prof. Stéphane Bordas, Director.
Extended FEM/ Meshless



Prof. Feodor Borodich
Theoretical/Nano mechanics, contact, adhesion



Prof. Pwt Evans
Contact mechanics, tribology



Dr. Paul Howson
Transcendental eigenvalue problems



Prof. Bhushan Karihaloo
Advanced materials, theoretical mechanics



Prof. David Kennedy
Eigenvalue problems, advanced numerical methods



Dr. Pierre Kerfriden
Multiscale, model order reduction, fracture



Dr. Siva Kulasegaram
Meshless methods



Prof. Ray Snidle
Contact mechanics, tribology



Dr. Lars Beex
Multiscale methods



Dr. Hanxing Zhu
Theoretical mechanics, cellular materials

The institute

- 6 professors, 6 lecturers/senior lecturers
- 10 post-doc fellows
- 17 PhD students
- ~ £1.0M funding annually



Theoretical & Computational

Tribology & Contact Mechanics

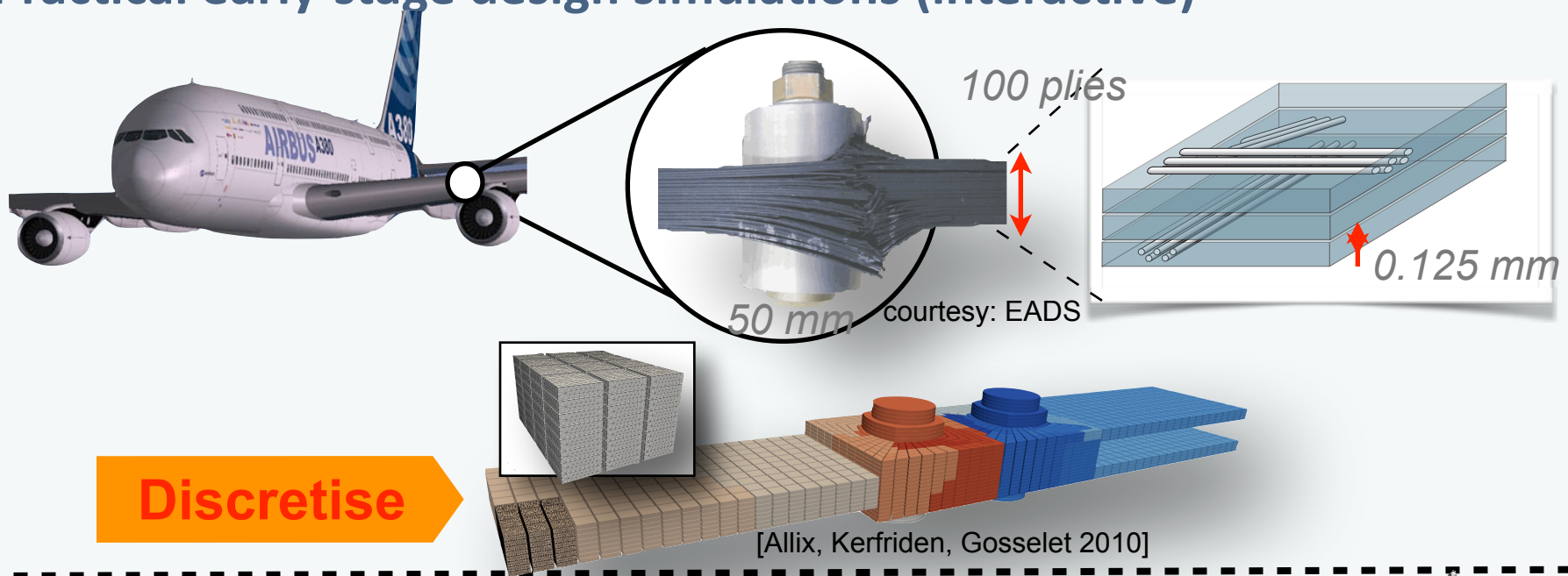
Experiments

Theory

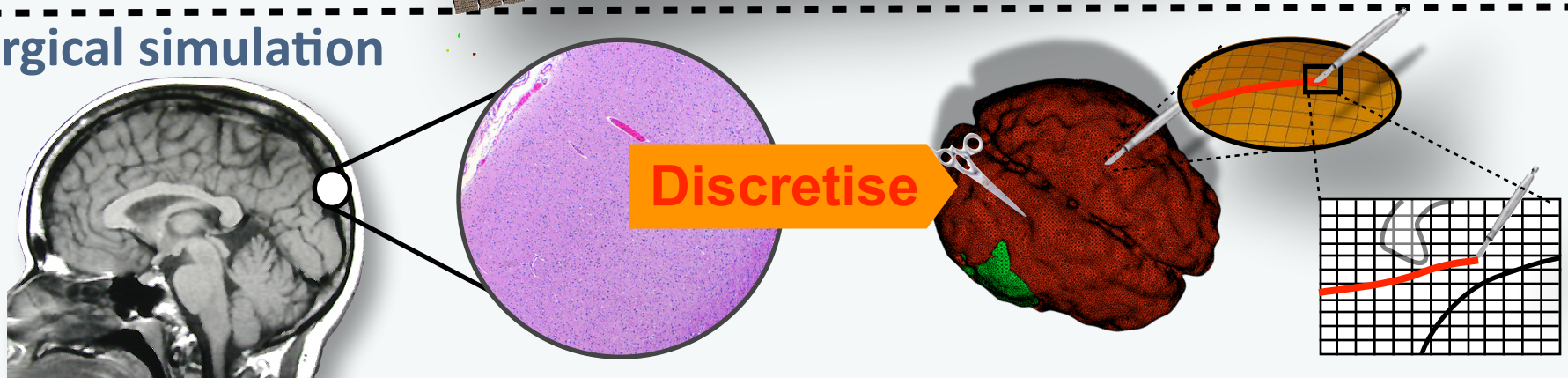
Computational Mechanics

Motivation: multiscale fracture of engineering structures and materials

Practical early-stage design simulations (interactive)



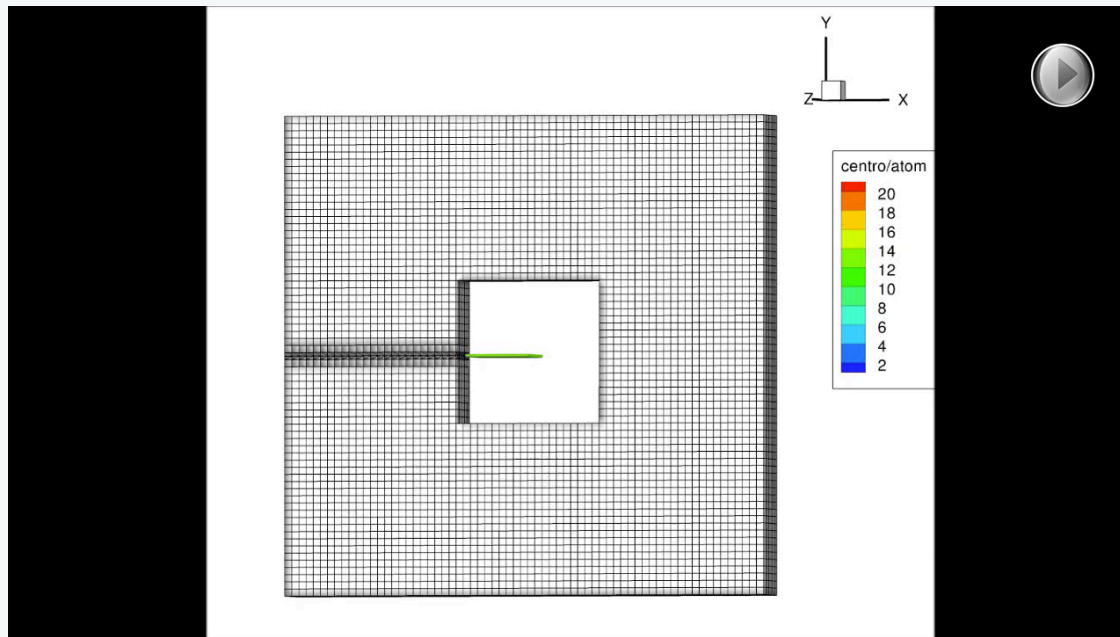
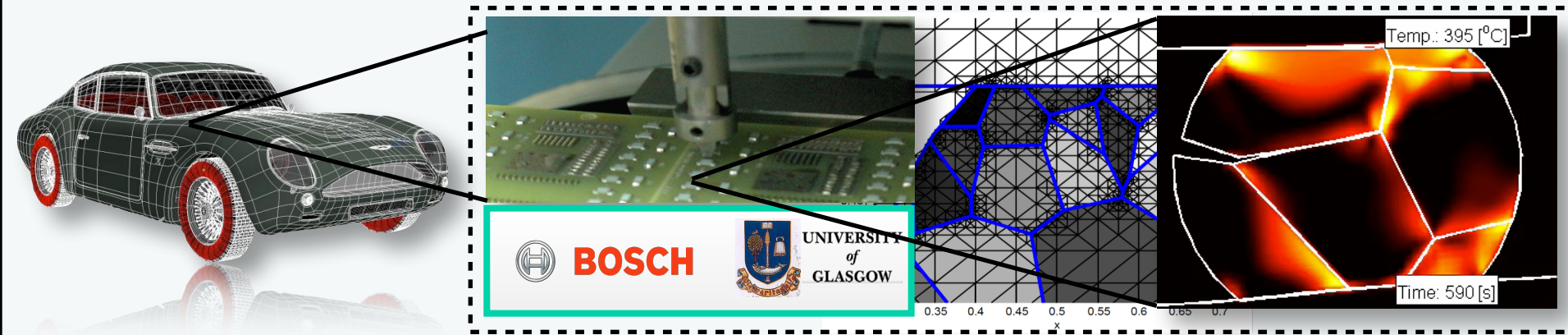
Surgical simulation



- Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

Motivation: multiscale fracture of engineering structures and materials

Solder joint durability (microelectronics), Bosch GmbH



Discretization

- ➡ partition of unity enrichment
- ✓ (enriched) meshless methods
- ✓ level sets
- ➡ isogeometric analysis
- ➡ implicit boundaries

Model reduction ¹²

- ✓ multi-scale & homogenisation
- ✓ algebraic model reduction (using POD)
- ✓ Newton-Krylov, “local/global”, domain decomposition

Error control

- ✓ XFEM: goal-oriented error estimates
 - ▶ used by CENAERO (Morfeo XFEM)
- ✓ meshless methods for fracture
- ✓ error estimation for reduced models

Part 0. An adaptive method for fracture - application to polycrystalline failure

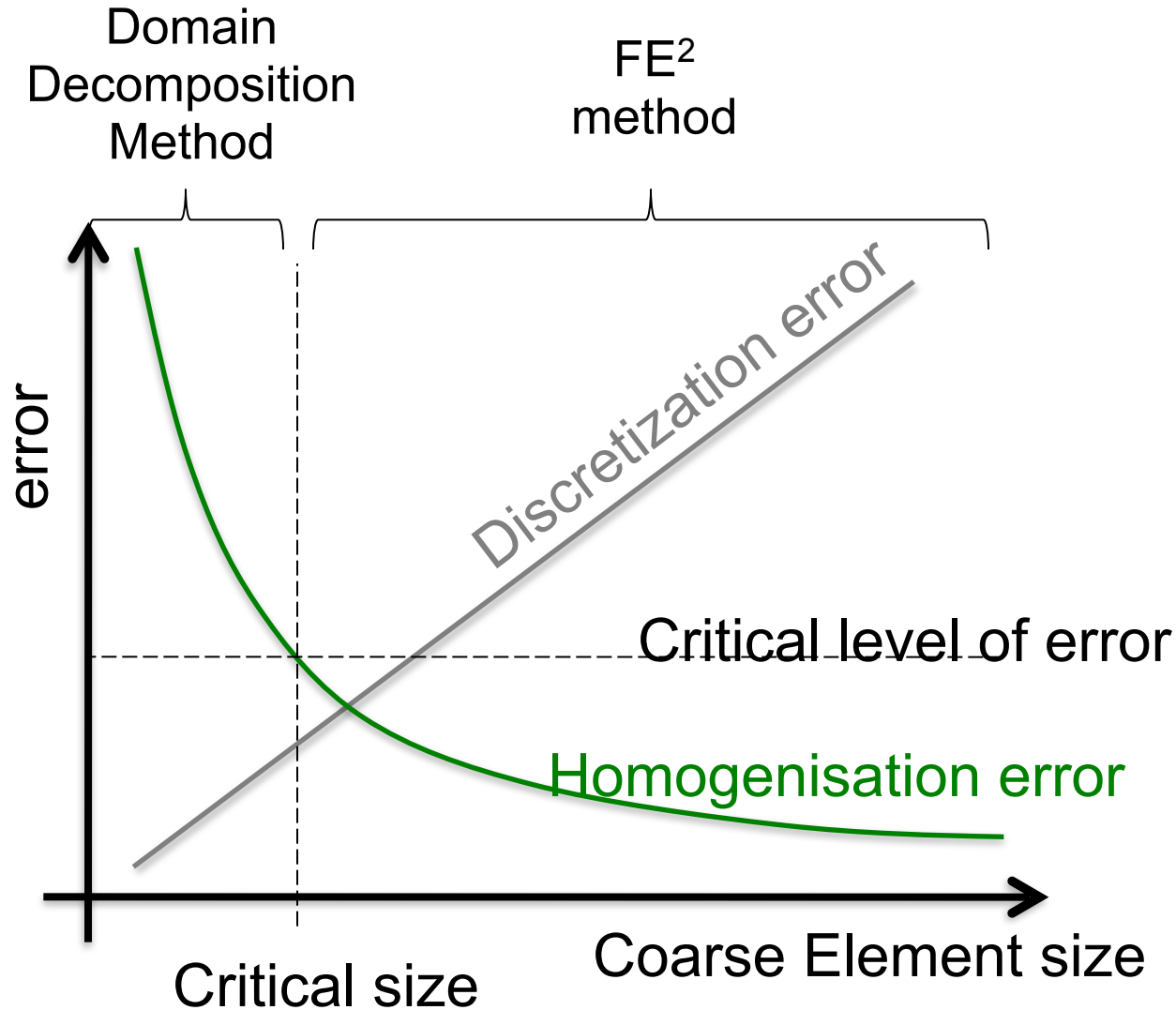
Ahmad Akbari, Pierre Kerfriden, Spaß



Adaptive method for fracture

- Introduction: Multiscale methods for Fracture
- Adaptive multiscale method
 - Strategy
 - Fine scale problem
 - Coarse scale problem
 - FE² method
 - Adaptive mesh refinement
 - Coupling fine and coarse discretisations
 - Results
 - L-shape problem
 - Notched bar under Uni-axial tension

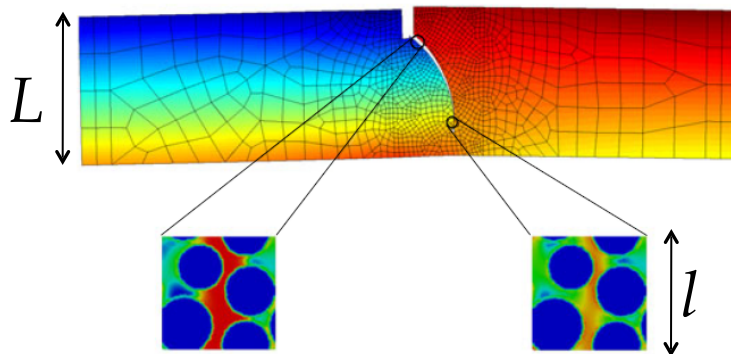
Error control in multiscale modelling



Multiscale methods for Fracture

■ Non-concurrent

Damage zone is modelled by a macroscopic cohesive crack that homogenises the failure zone.

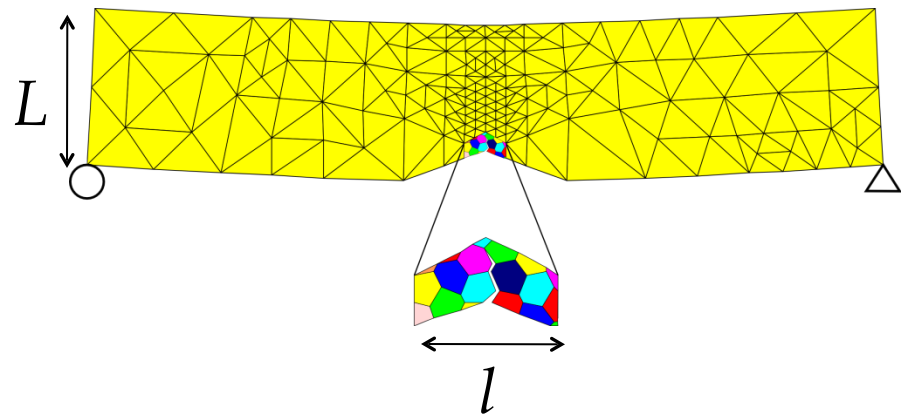


V.P. Nguyen 2012

$$L/l \gg 1$$

■ Concurrent

Damage zone is modelled directly at the microscale and coupled to the coarse scale.

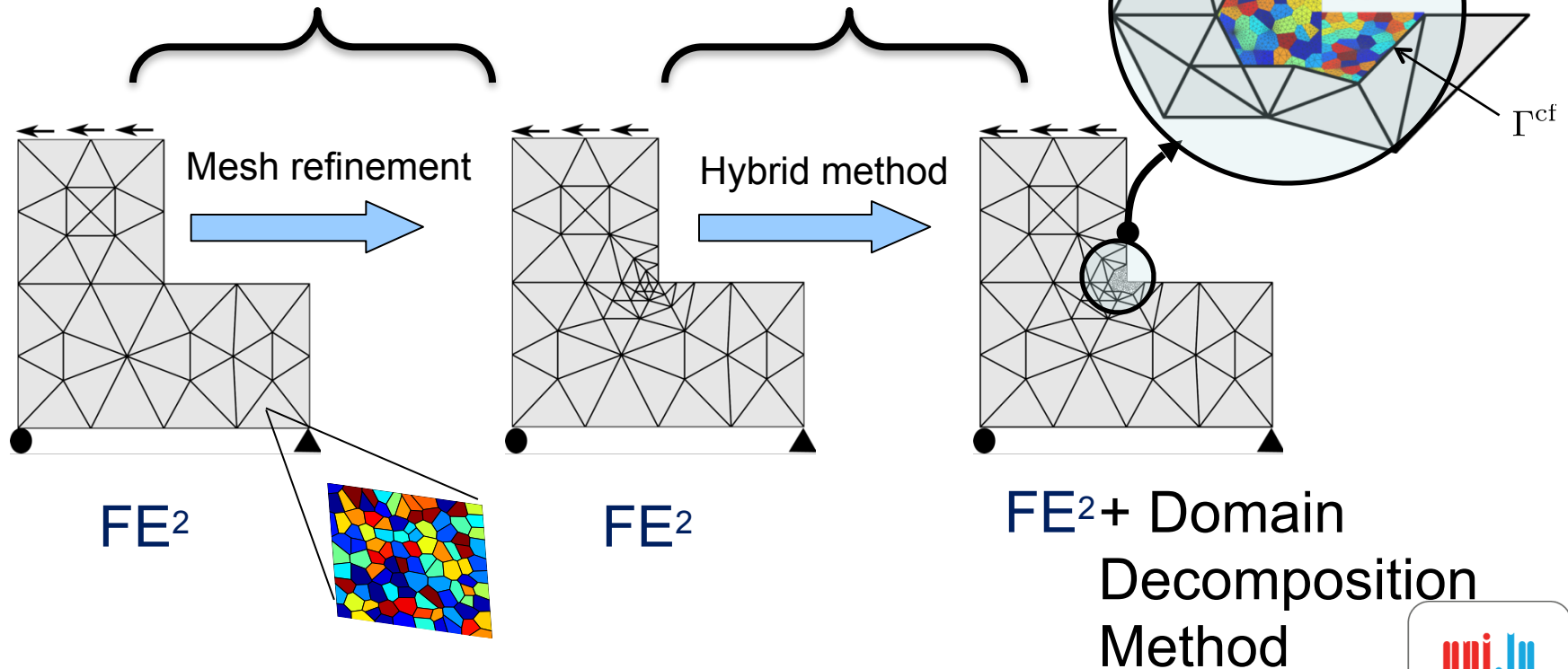


$$L/l > 1$$

Adaptive multiscale method: A Concurrent approach

➤ Strategy:

- control the coarse scale discretization error
- control the modelling error



Fine Scale: micro-structure

➤ Microscale problem:

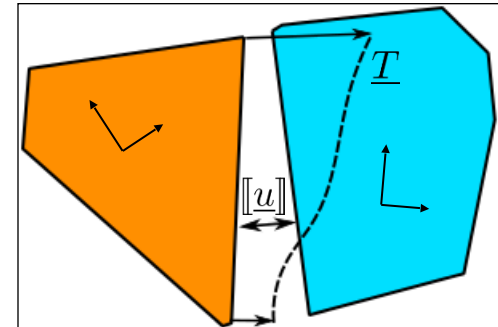
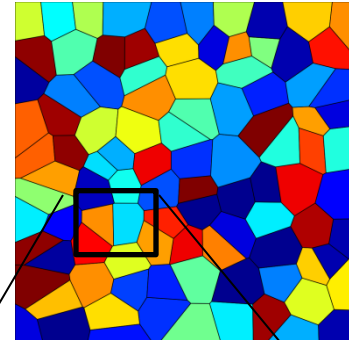
$$\int_{\Omega/\Gamma_c} \boldsymbol{\sigma}(\mathbf{u}) : \delta \boldsymbol{\varepsilon} \, d\Omega + \int_{\Gamma_c} \mathbf{T} \cdot \llbracket \delta \mathbf{u} \rrbracket \, d\Omega = \int_{\partial\Omega} \mathbf{f} \cdot \delta \mathbf{u} \, d\Gamma$$

■ Orthotropic grains

$$\forall \mathbf{x} \in \Omega/\Gamma_c, \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}$$

■ Cohesive interface

$$\forall \mathbf{x} \in \Gamma_c, \quad \mathbf{T}|_t = T \left((\llbracket \mathbf{u} \rrbracket|_T)_{T \leq t} \right)$$



Coarse Scale

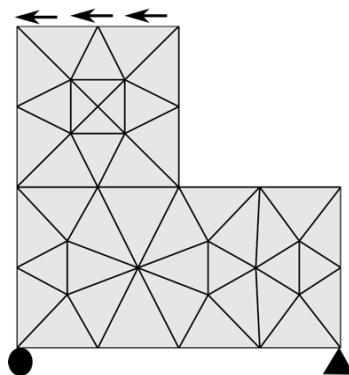
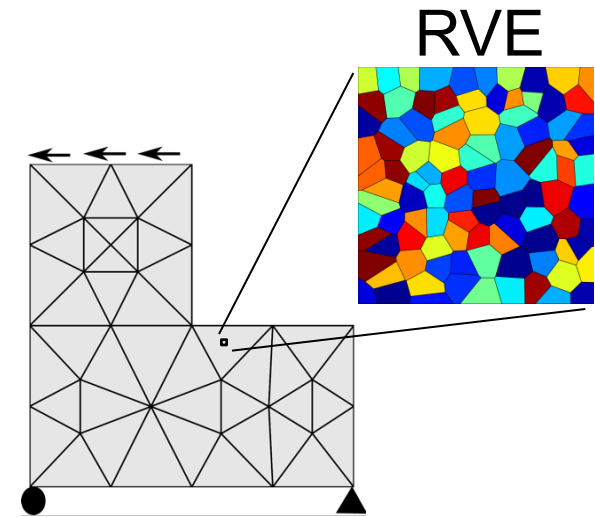
➤ Macroscale problem:

■ FE² Method

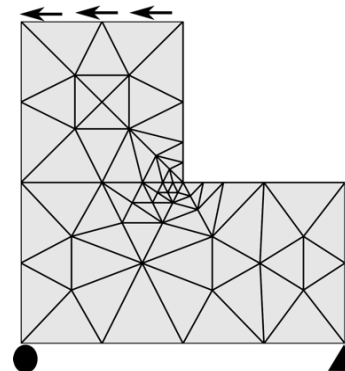
Based on averaging theorem
(computational homogenisation)

■ Adaptive mesh refinement

Error estimation by Zienkiewicz-Zhu-type recovery technique

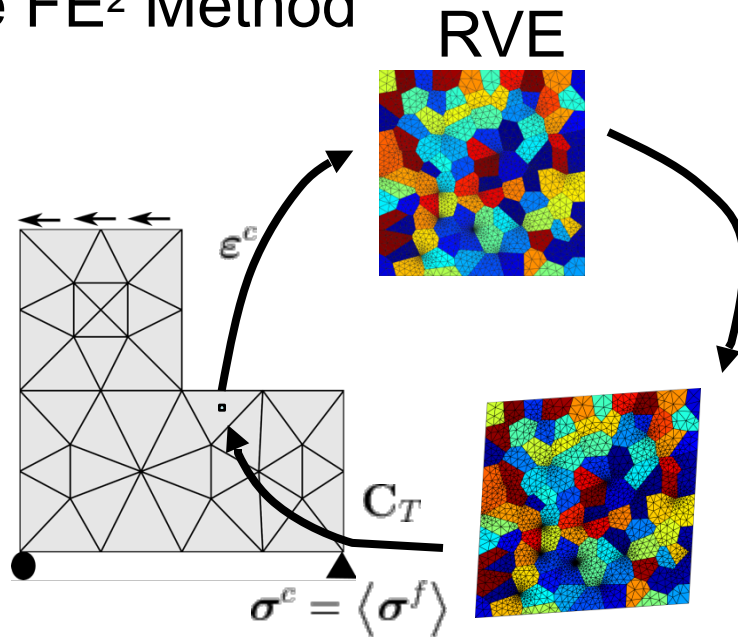


Mesh refinement

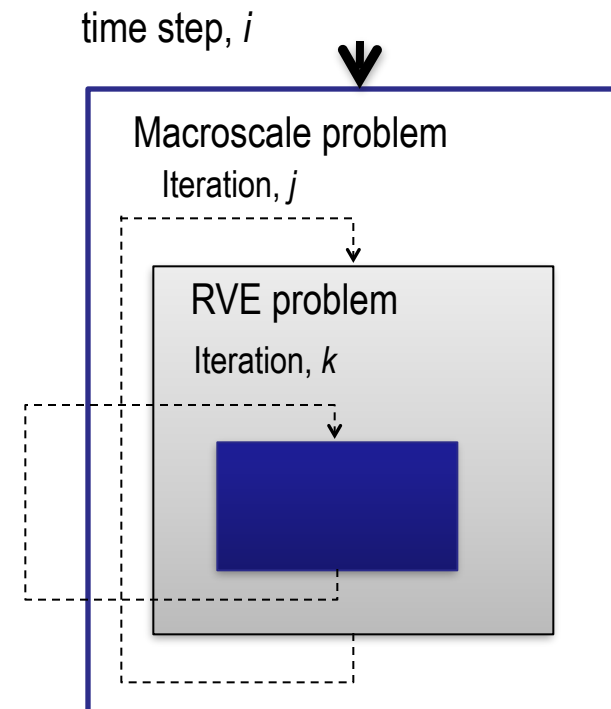


Coarse Scale: FE2

■ The FE² Method



❖ Shortcoming of the FE² Method :



Lack of scale separation

RVE cannot be found in the **softening regime**

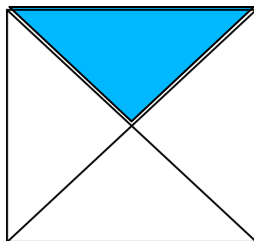
Coarse Scale: Adaptive mesh refinement

➤ Coarse scale Adaptive mesh refinement

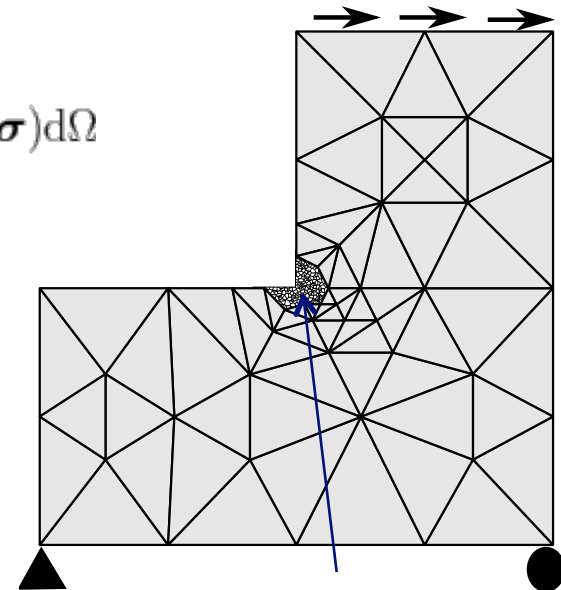
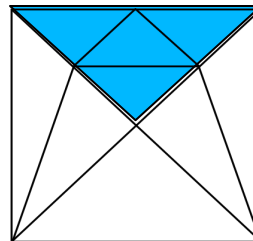
- Error estimation by Zienkiewicz-Zhu-type recovery technique

$$\|e\| = \int_{\Omega_c} (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}) : \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} \Big|_{\mathbf{u}^c} \right)^{-1} : (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}) d\Omega$$

Element to refine



Refined mesh



Error due to the
discretisation of Ω^f
neglected

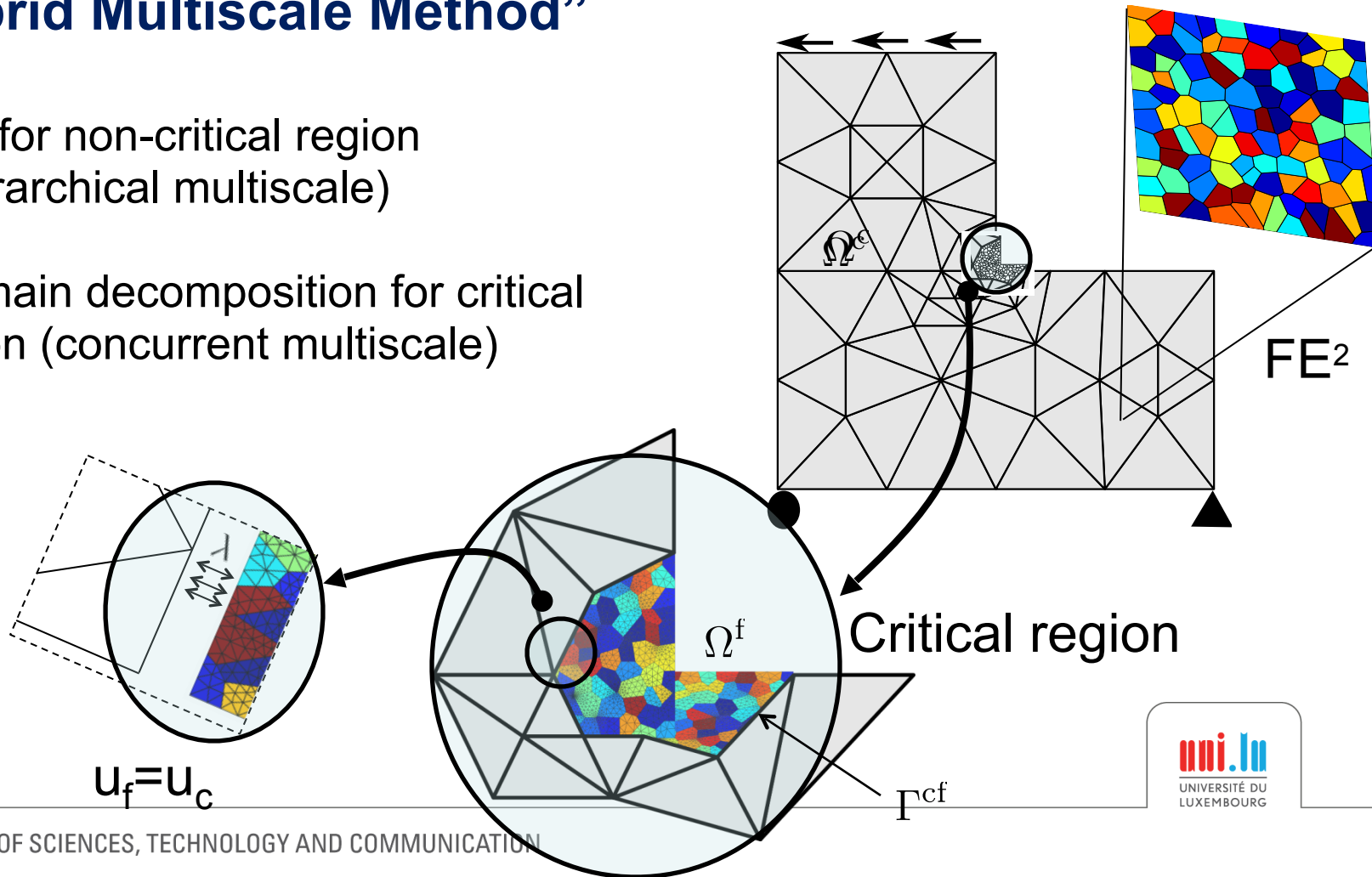
- Convergence criterion: $\frac{\|e\|}{\|\sigma\|} < Tol$

Fine-Coarse scales Coupling

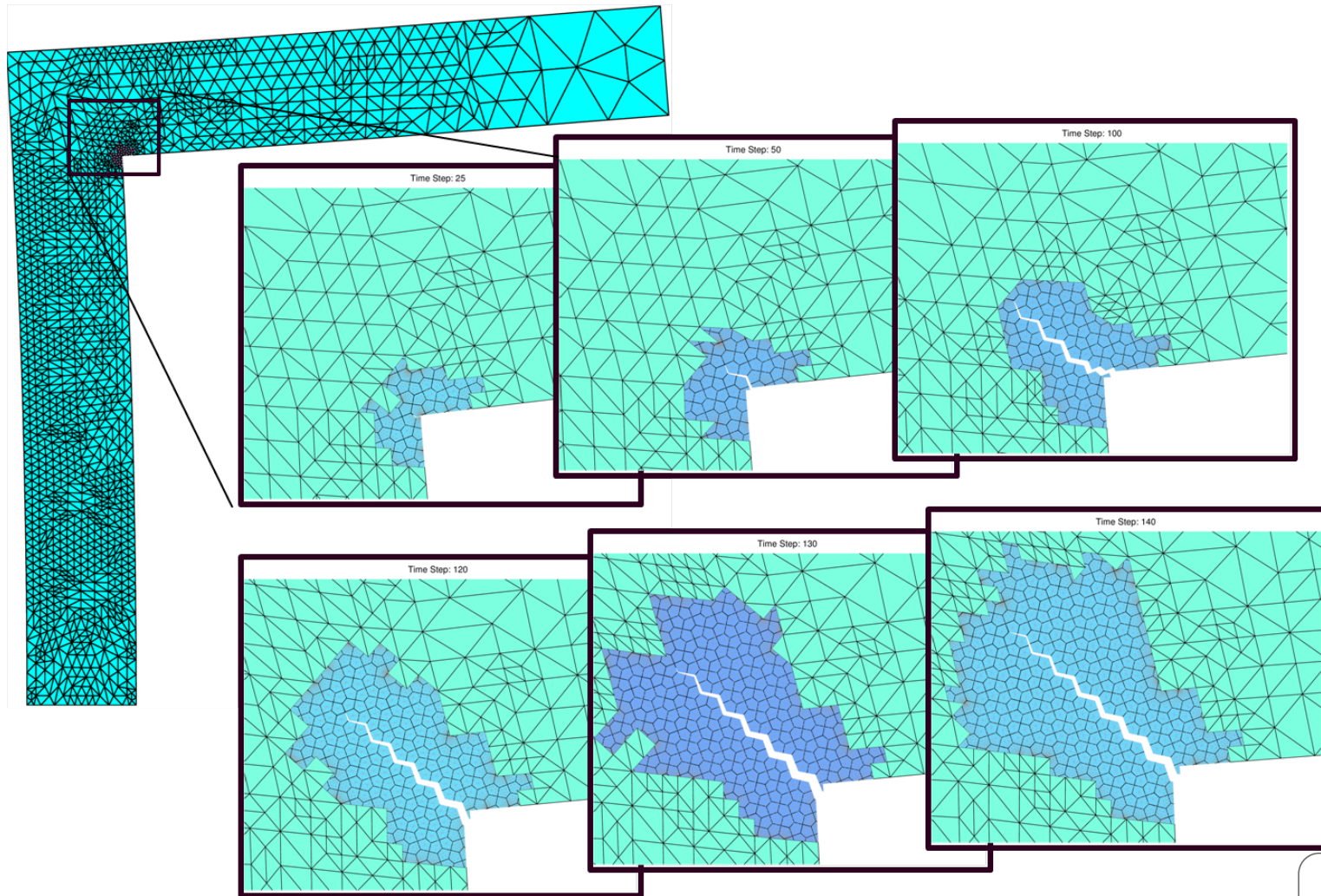
What is the solution for the FE^2 shortcoming:

“Hybrid Multiscale Method”

- FE^2 for non-critical region (hierarchical multiscale)
- Domain decomposition for critical region (concurrent multiscale)

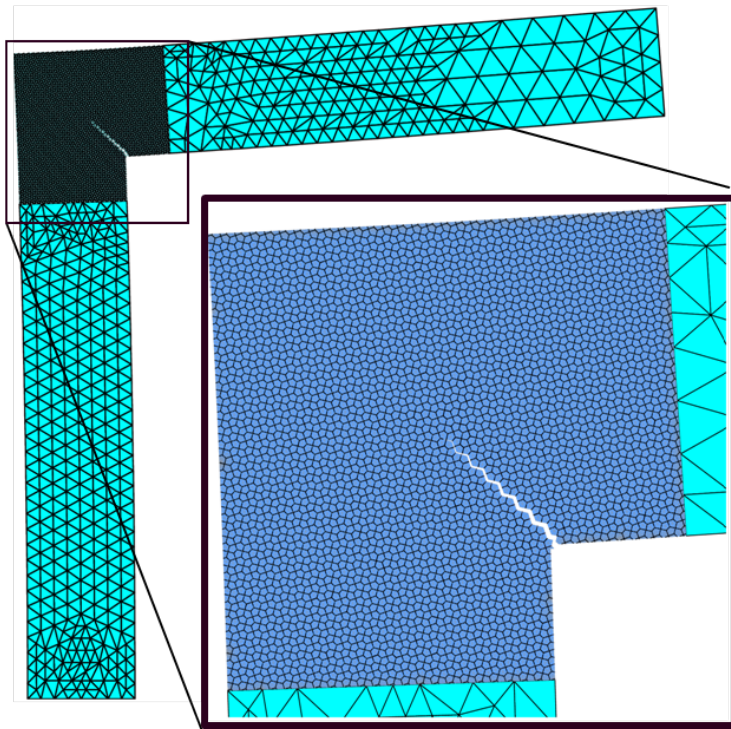


Results: L-shape

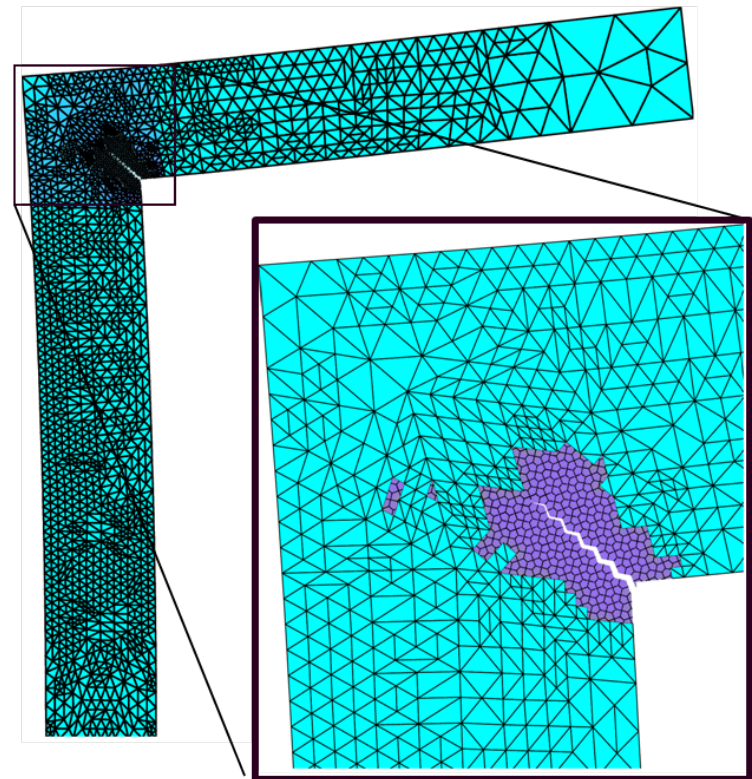


Results: L-shape

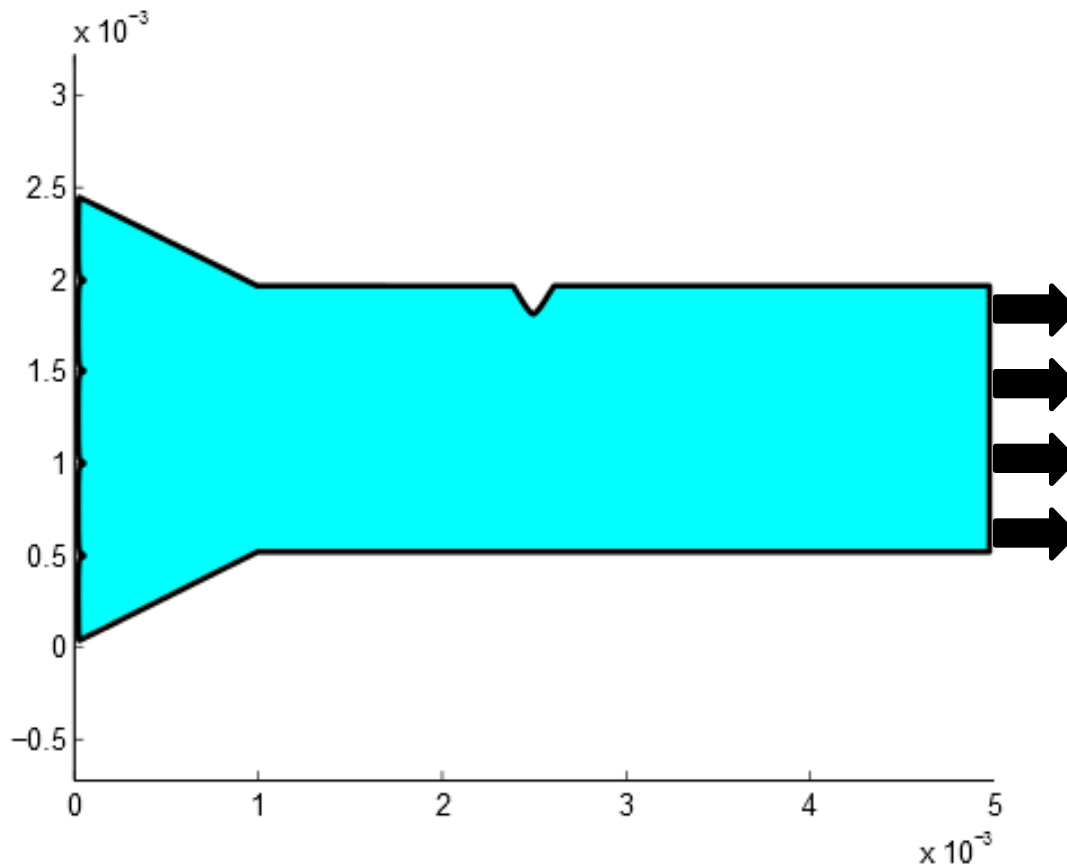
Direct Numerical Solution



Adaptive Multiscale method



Results: uni-axial tension

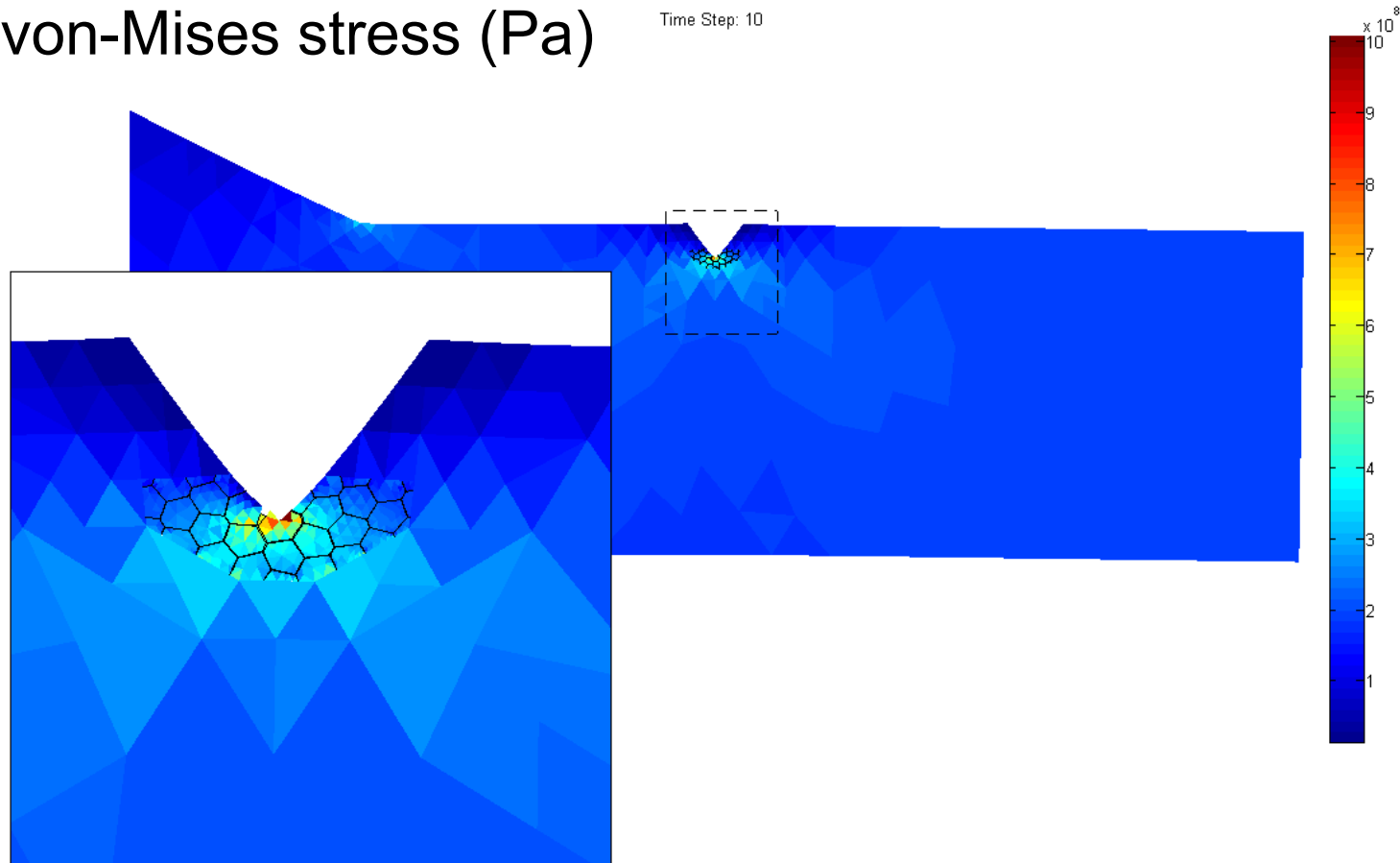


❖ Sizes are in mm

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 10

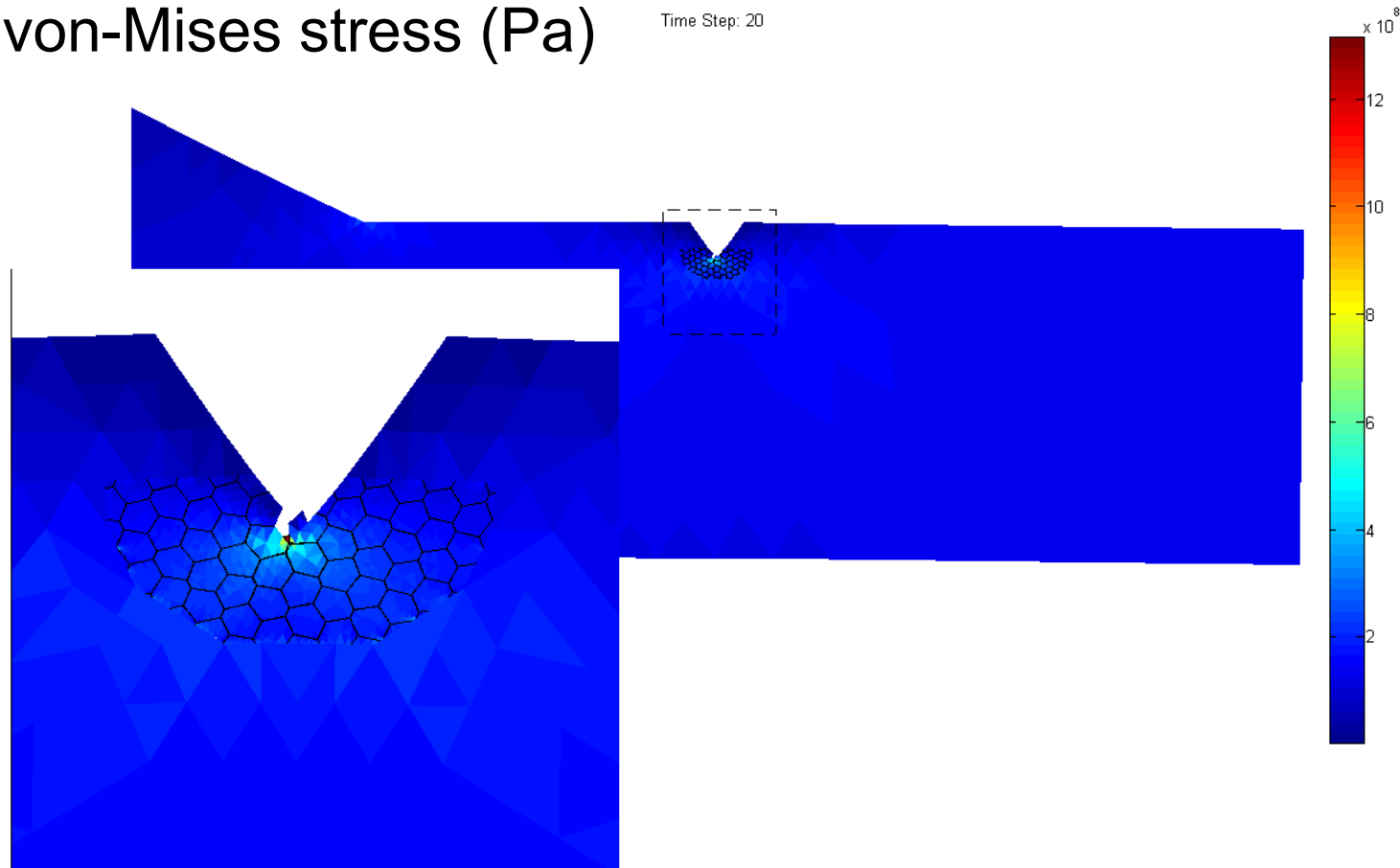


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 20

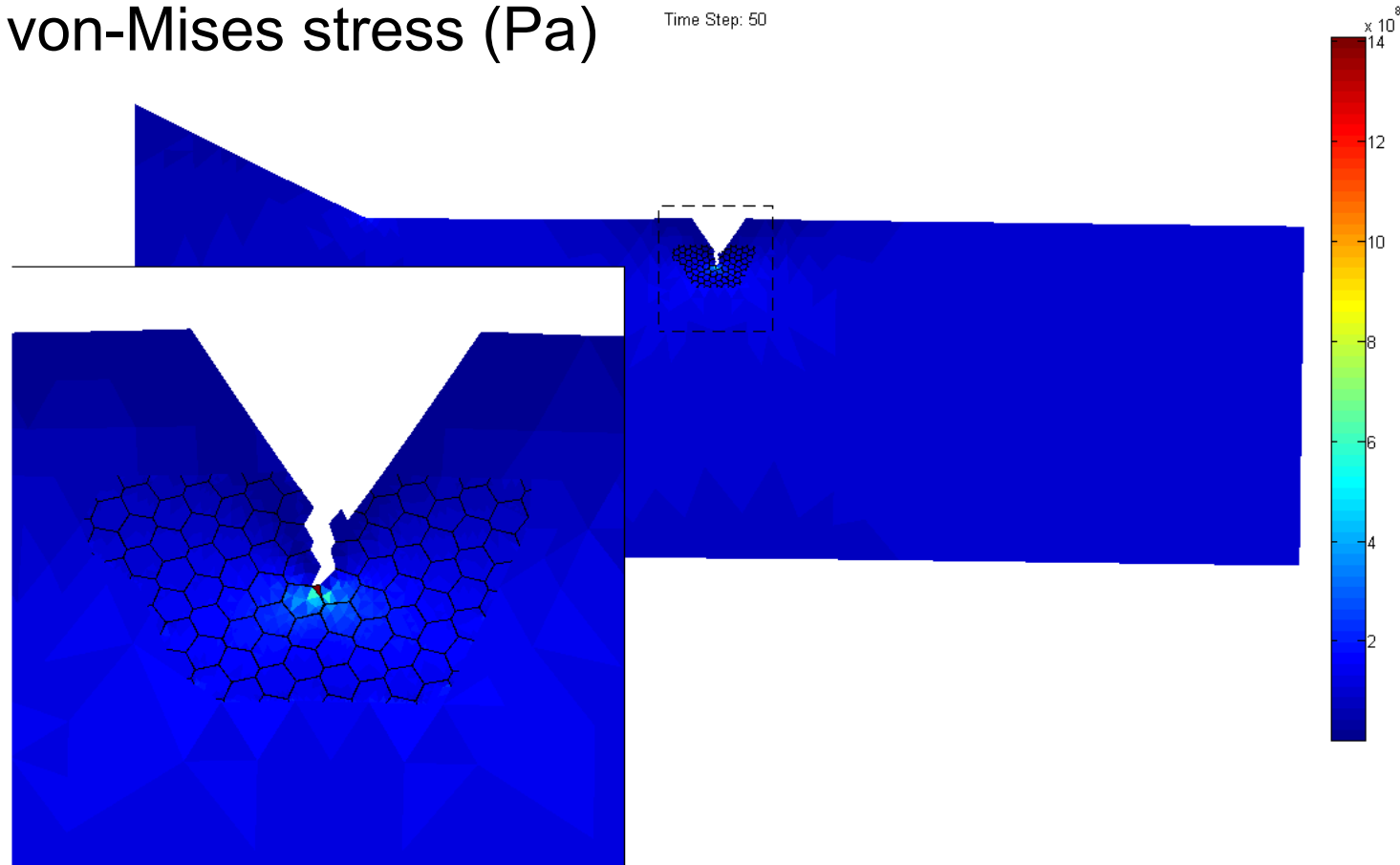


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 50

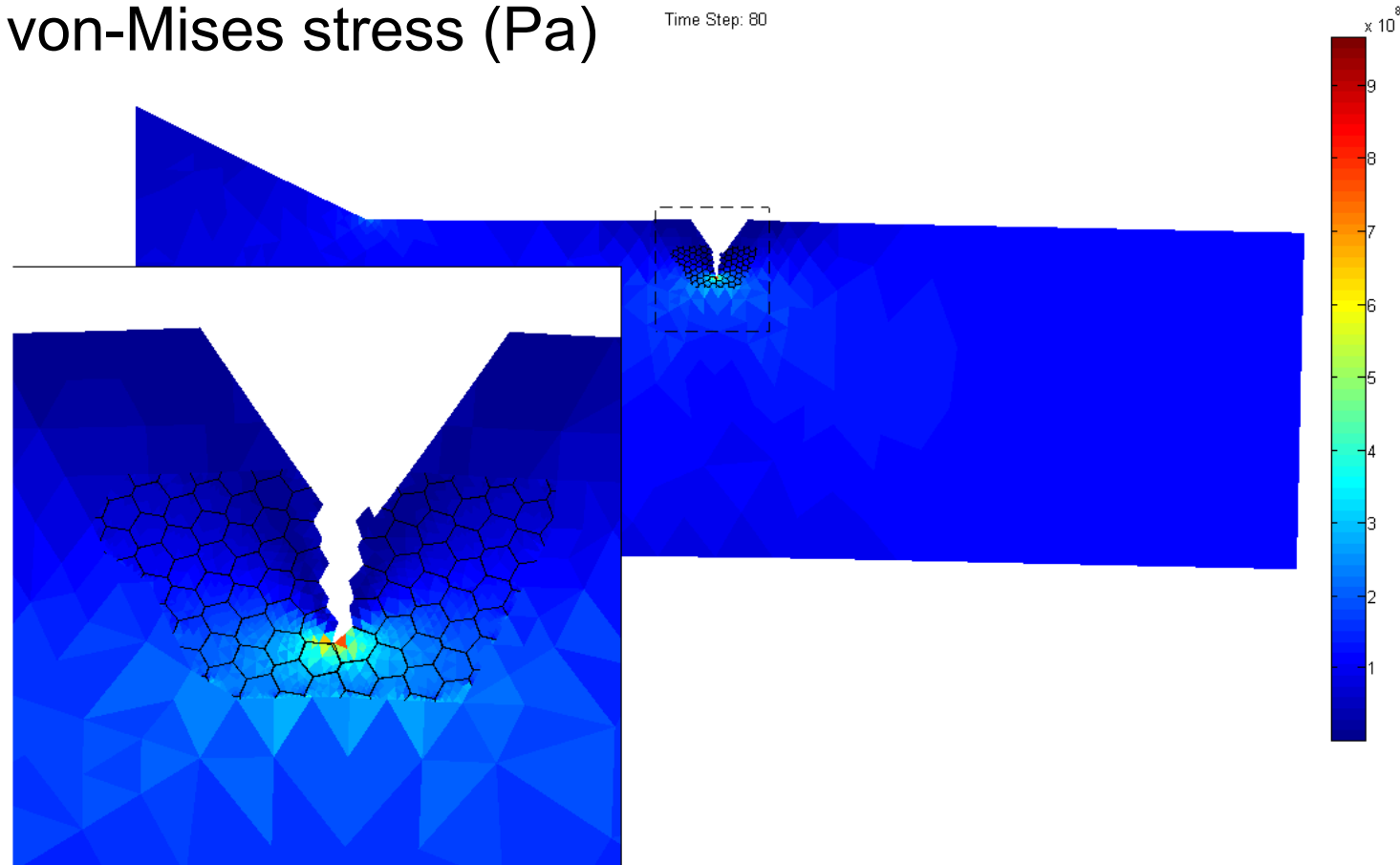


❖ 100X (magnification of displacement)

Results: uni-axial tension

von-Mises stress (Pa)

Time Step: 80

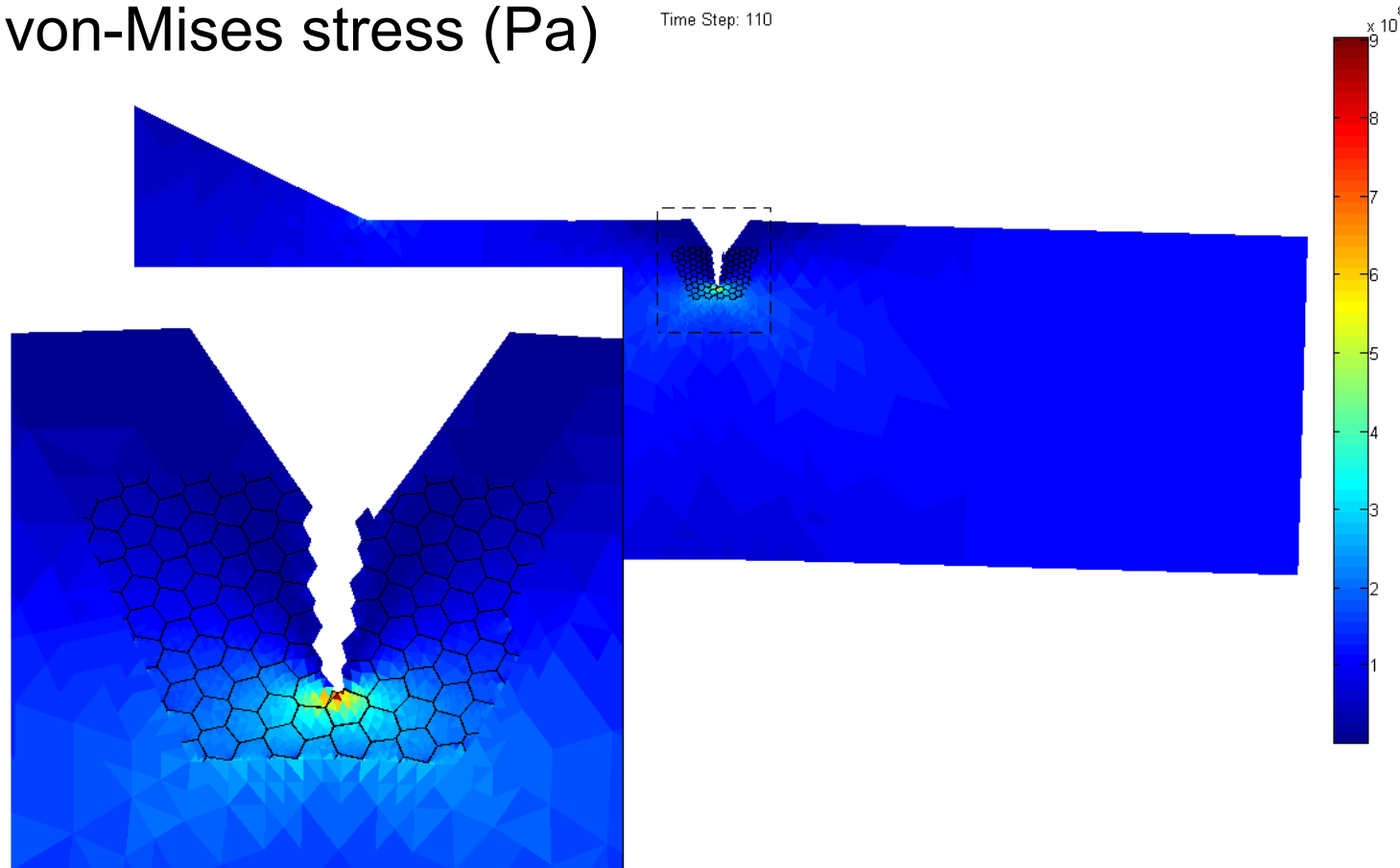


❖ 100X (magnification of displacement)

Results: uni-axial tension

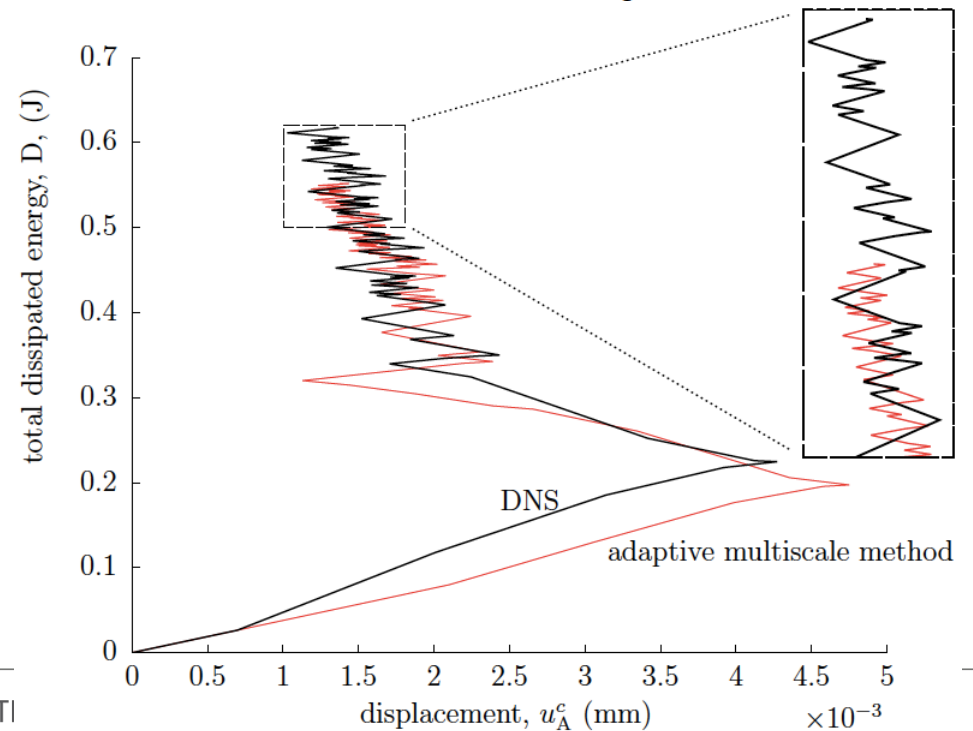
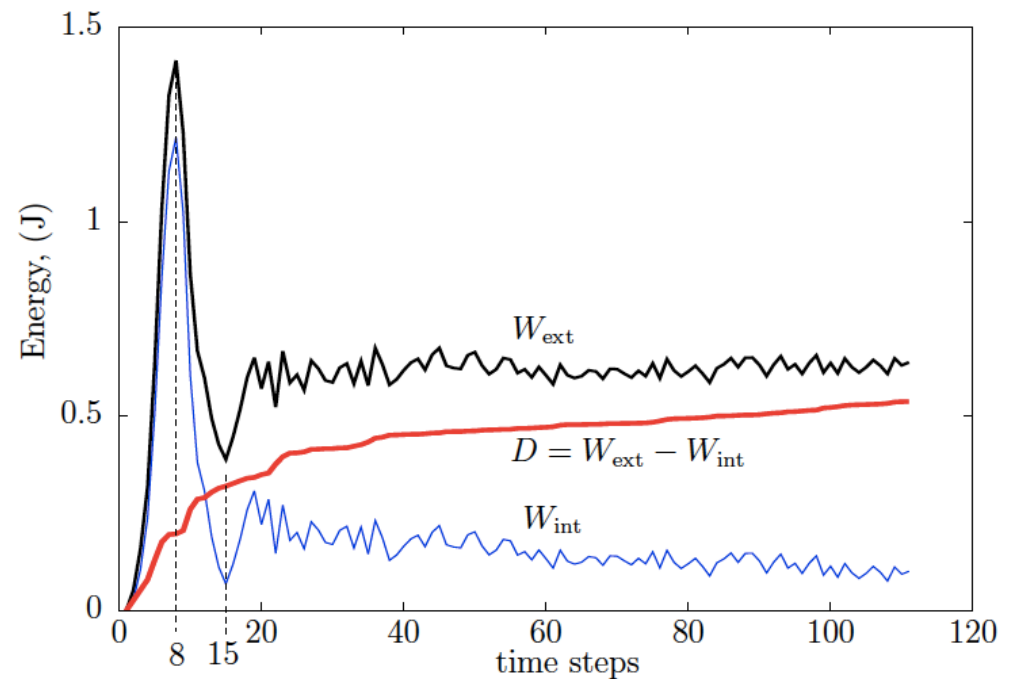
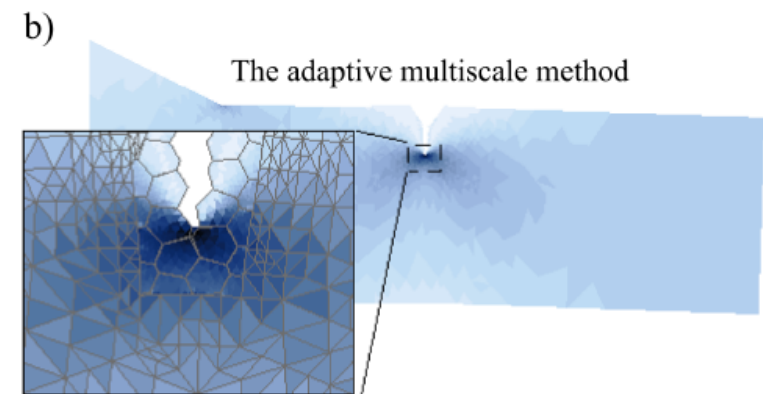
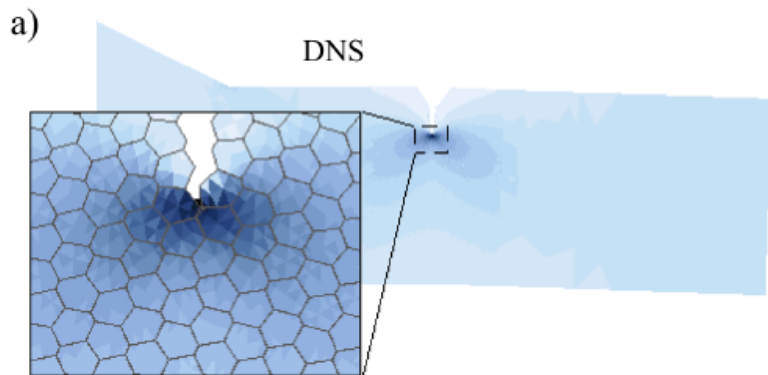
von-Mises stress (Pa)

Time Step: 110

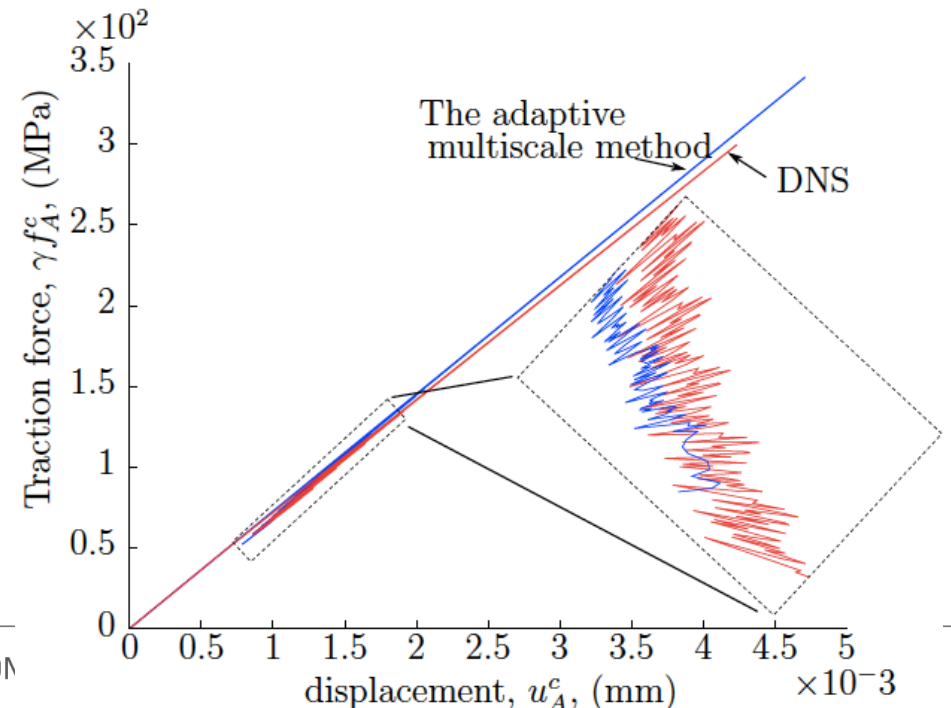
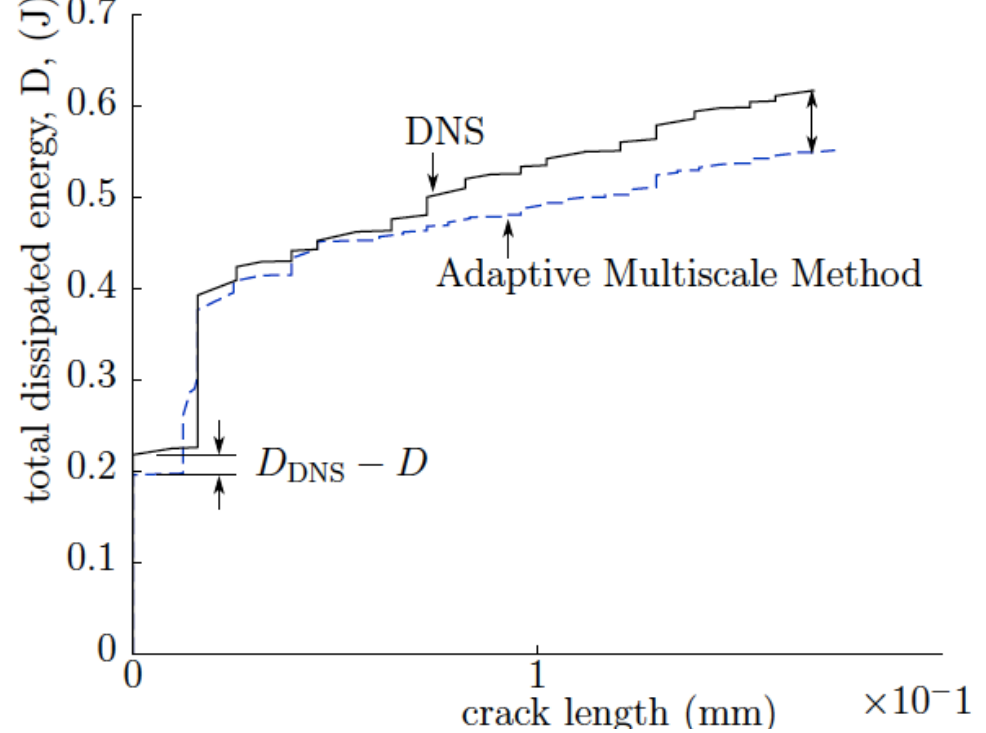
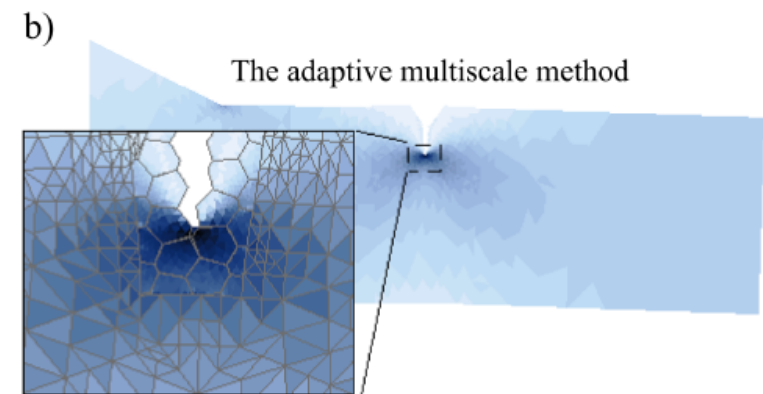
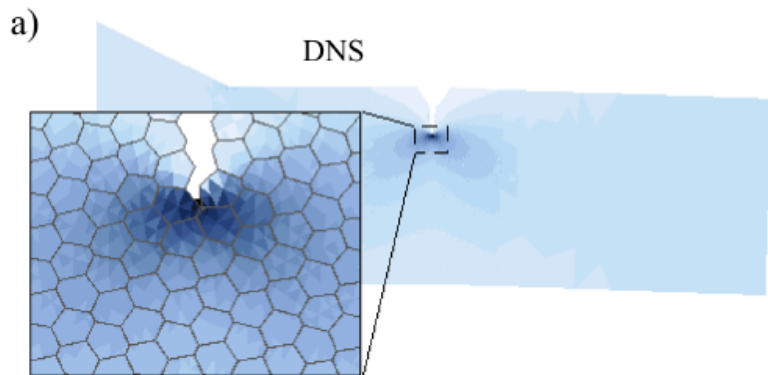


❖ 100X (magnification of displacement)

Verification



Verification



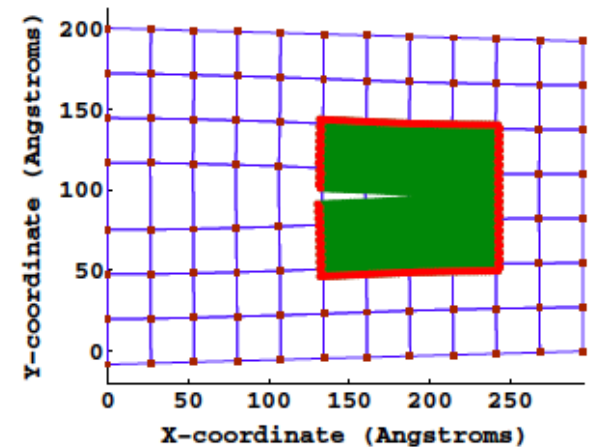
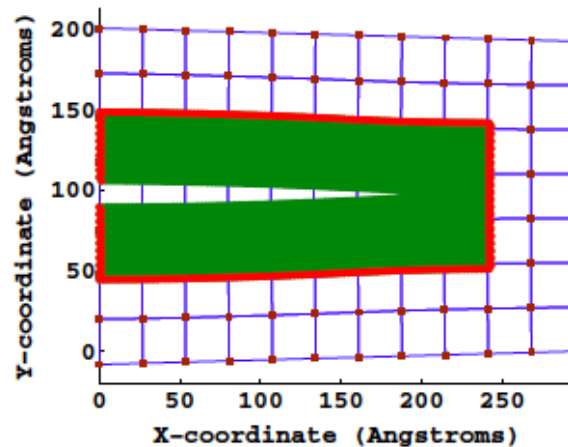
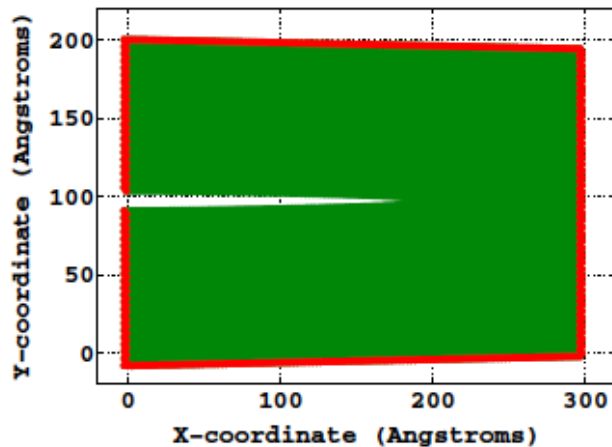
Adaptive Multiscale Method

An adaptive multiscale method was developed for discrete fracture in polycrystalline materials:

- An unstructured mesh is used for the coarse scale problem
- A local arc-length was used to control crack speed in the fully resolved region.
- A recovery based error indicator was employed to limit discretization error at each time step.

Perspectives

- coarsening once the crack is open
- molecular dynamics at the fine scale



- real-life problems! :)
- coupling with algebraic model reduction (POD)

- Part I.** Streamlining the CAD-analysis transition
- Part II.** Some advances in enriched FEM
- Part III.** Application to H cutting of Si wafers
- Part IV.** Interactive cutting sim.

erc

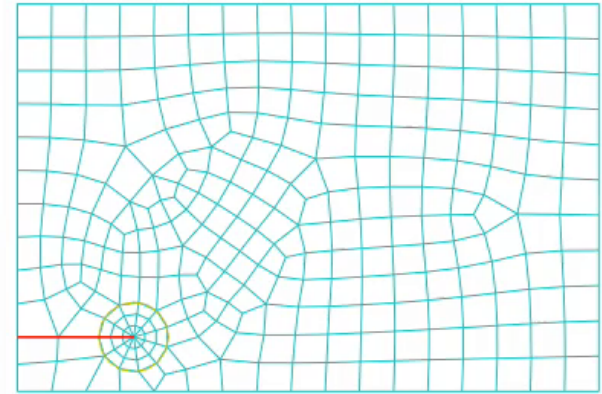
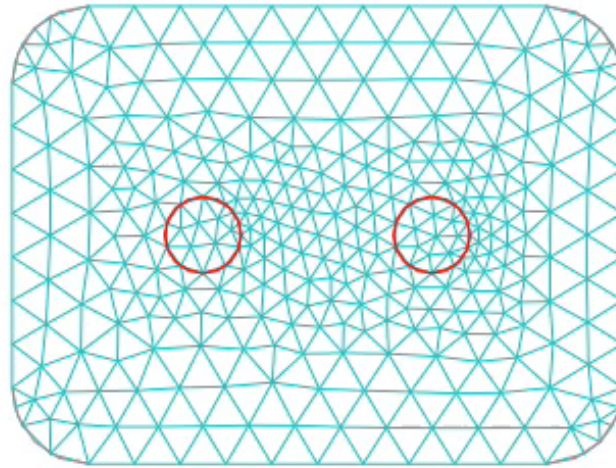
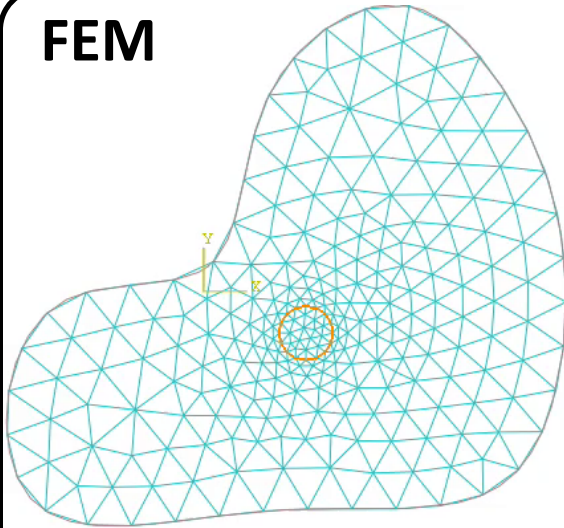
Part I. Streamlining the CAD-analysis transition

Coupling, or decoupling?

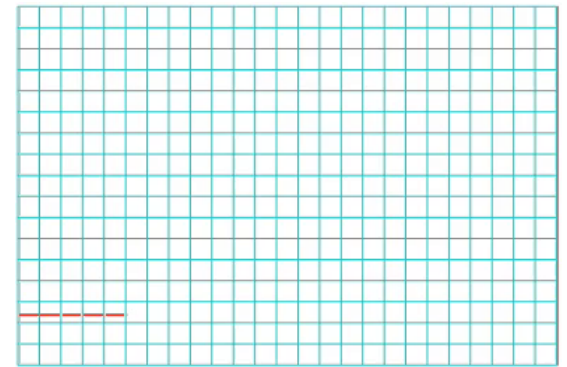
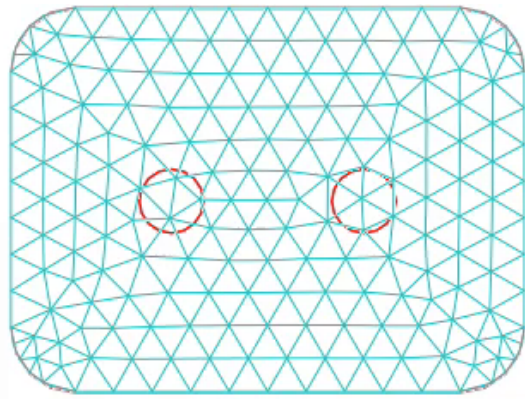
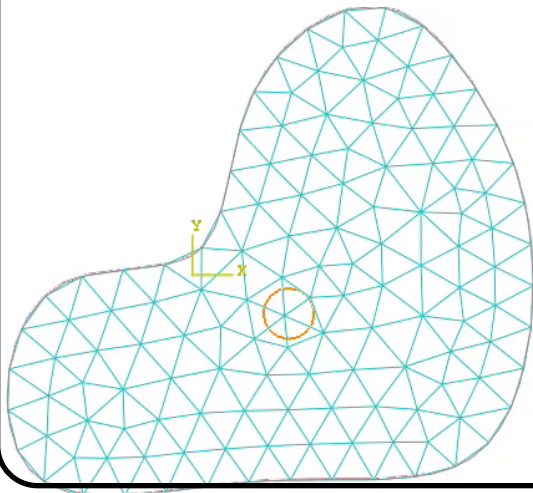


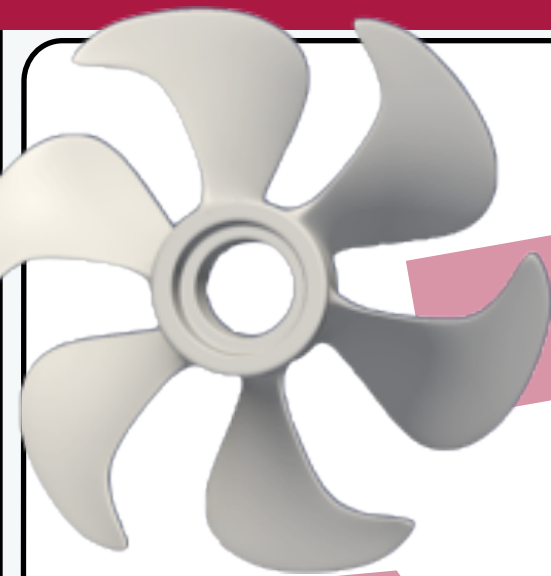
Motivation: free boundary problems - mesh burden

FEM



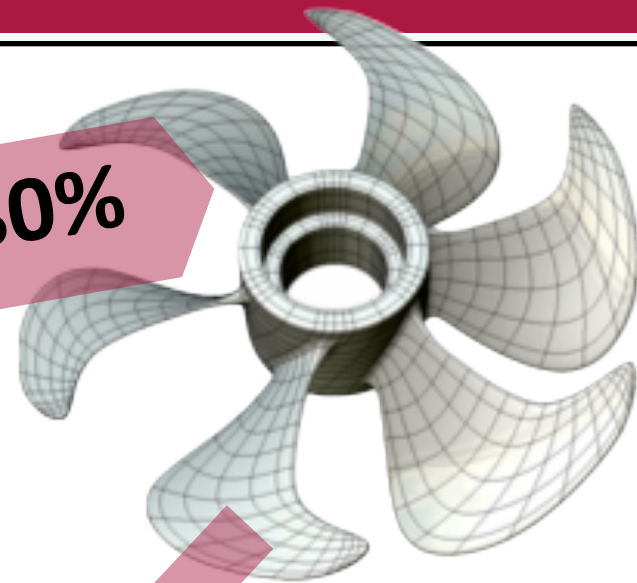
XFEM





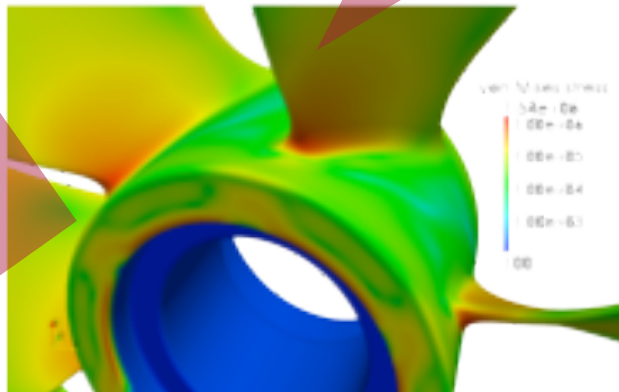
mesh

80%



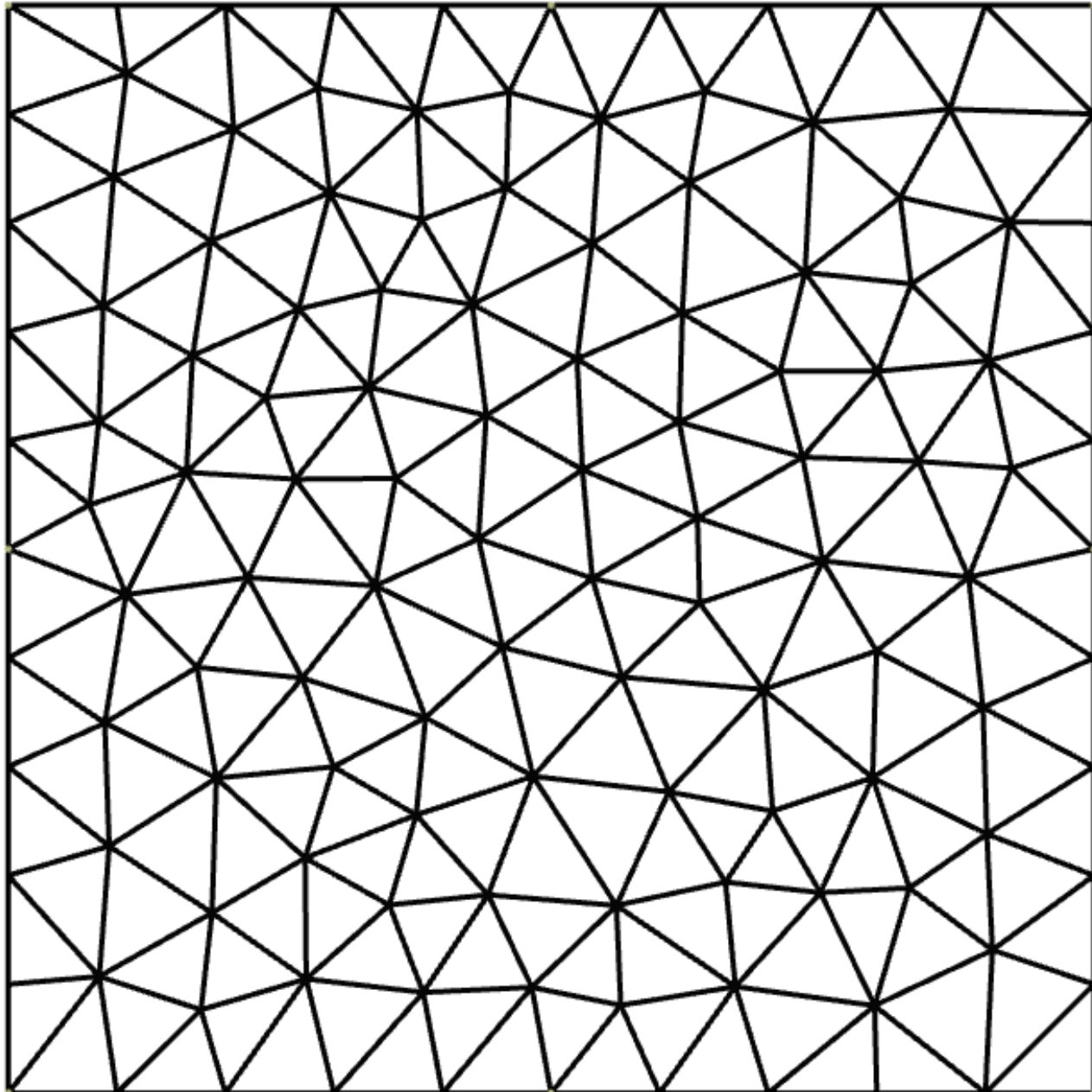
iterate

calculate
20%

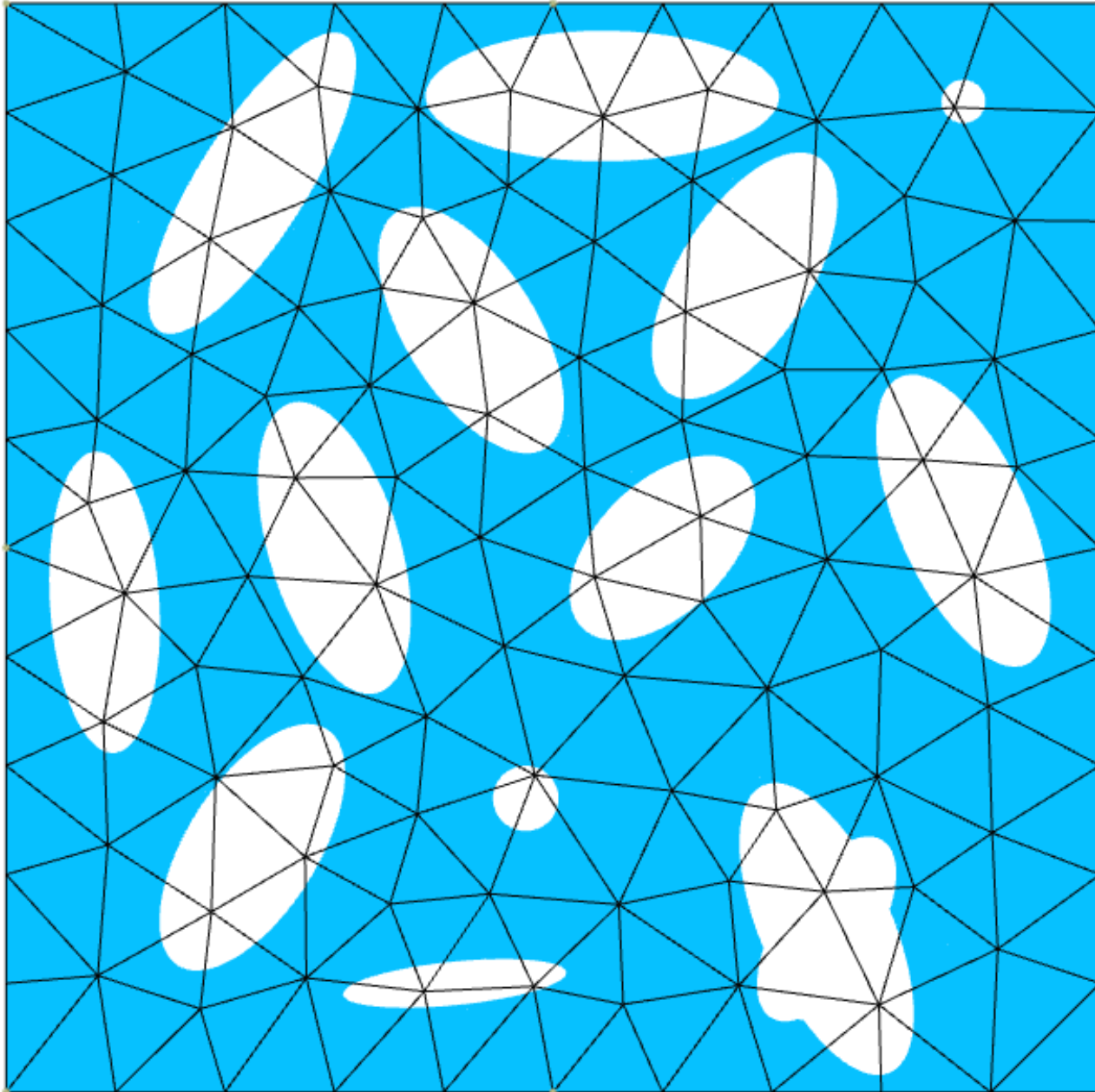


vM stress distribution

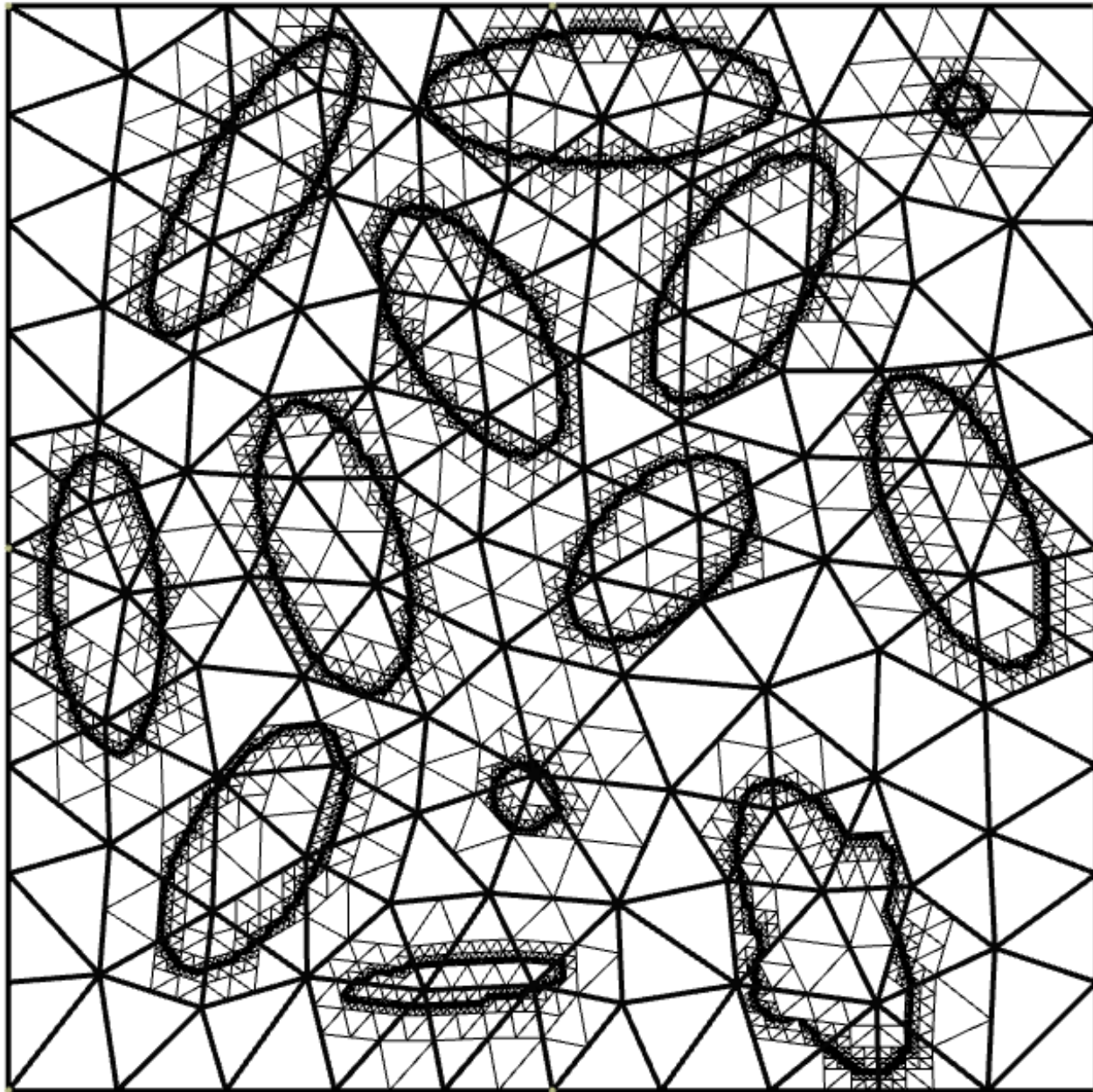
One would like to be able to use such a mesh



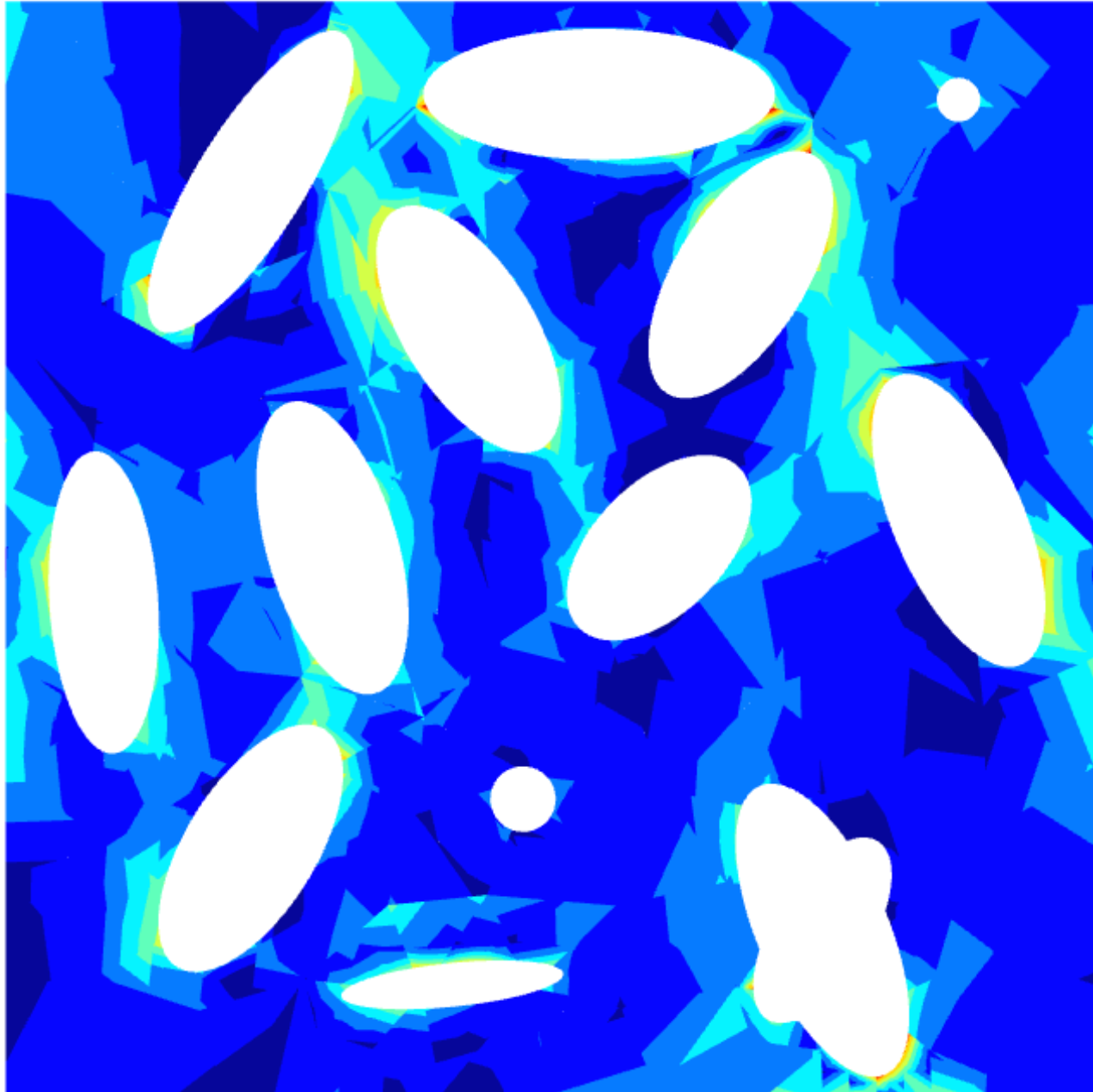
Superimpose the geometry onto an arbitrary background mesh



Compute interactions between the geometry and the mesh

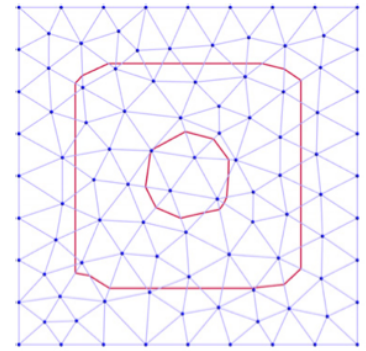


Perform the analysis

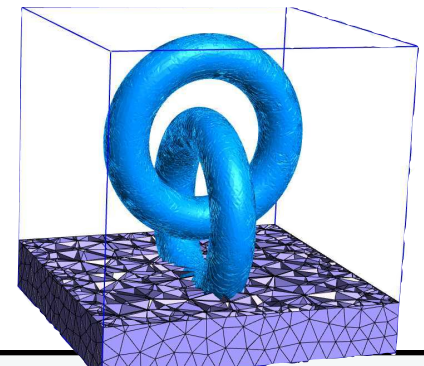
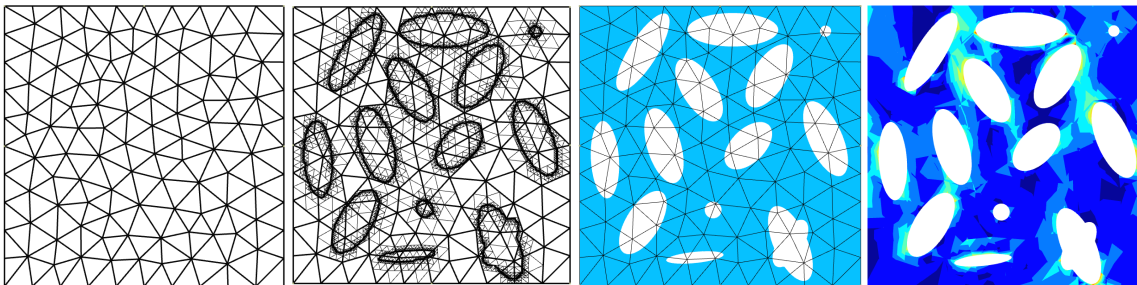


Paradigm 1: Separate field and boundary discretisation

- Immersed boundary method (Mittal, *et al.* 2005)
- Fictitious domain (Glowinski, *et al.* 1994)
- Embedded boundary method (Johansen, *et al.* 1998)
- Virtual boundary method (Saiki, *et al.* 1996)
- Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

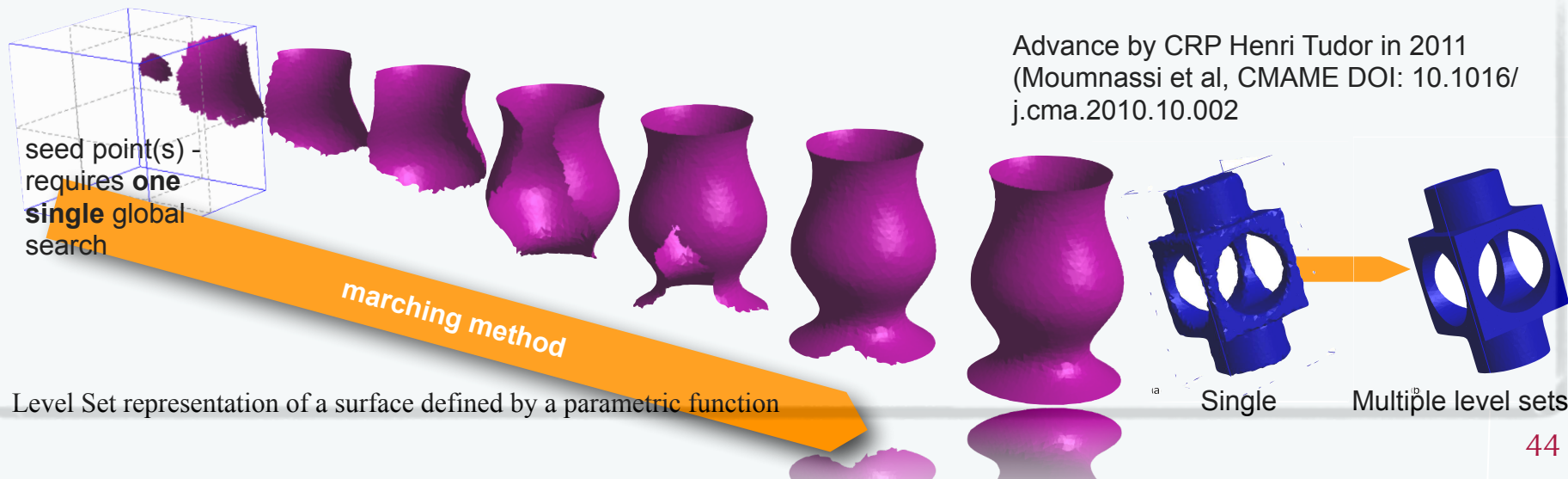
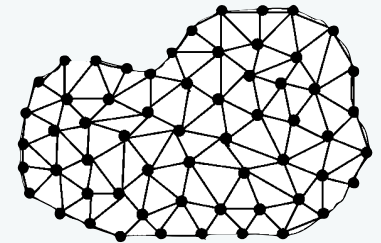
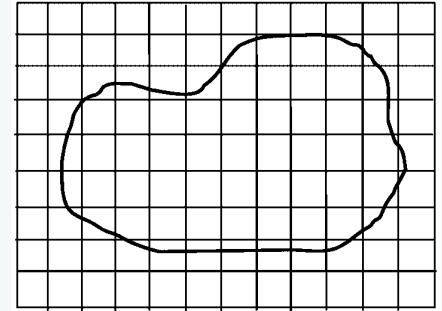


- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- Accuracy for complicated geometries? BCs on implicit surfaces?
- ➔ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi, *et al.* 2011)



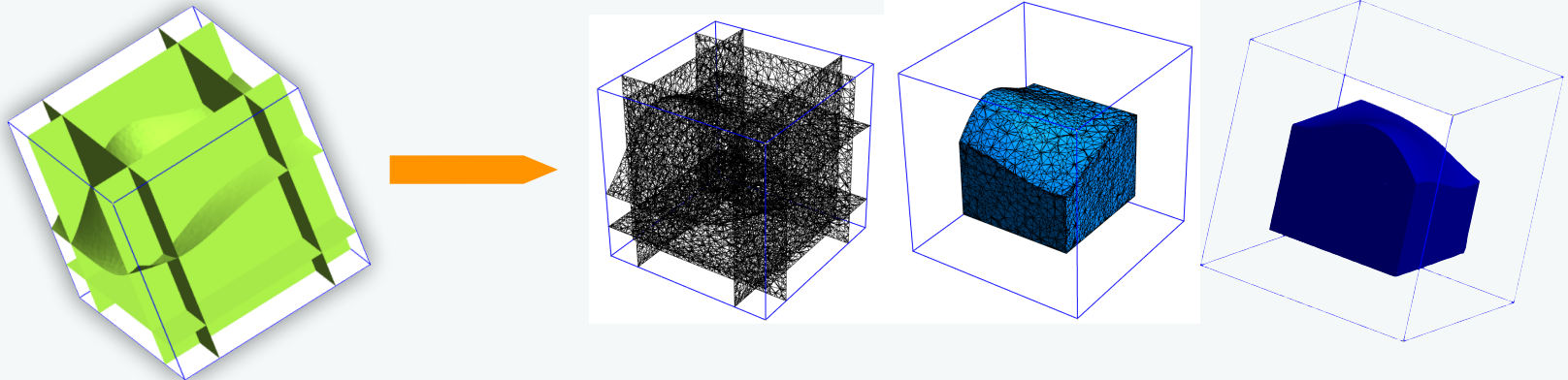
Objectives

- ▶ insert surfaces in a structured mesh
 - without meshing the surfaces (boundary, cracks, holes, inclusions, etc.)
 - directly from the underlying CAD model
 - model arbitrary solids, including sharp edges and vertices
- ▶ keep as much as possible of the mesh as the CAD model evolves, i.e. reduce mesh dependence of the implicit boundary representation
- ▶ maintain the convergence rates and implementation simplicity of the FEM

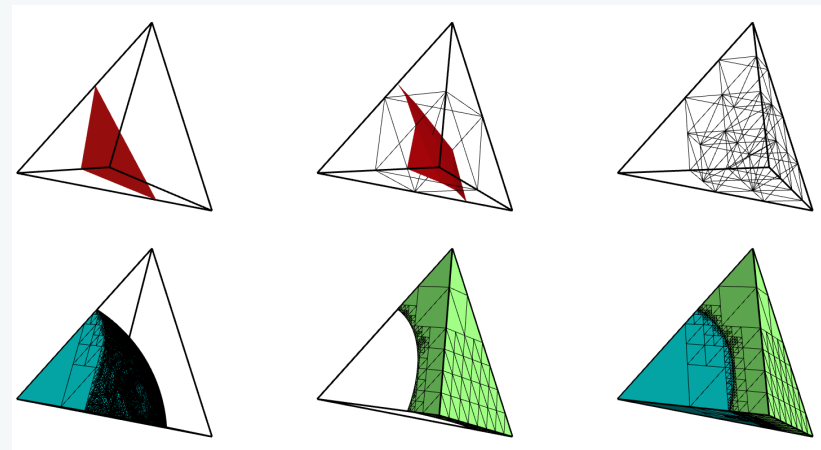
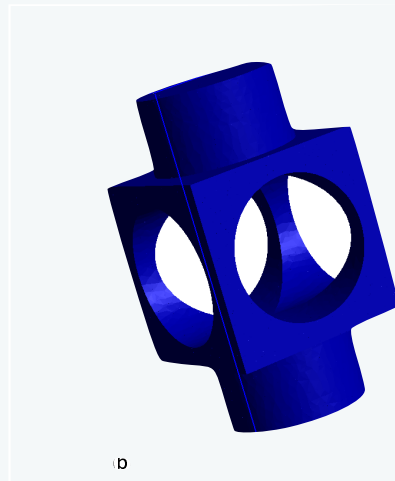
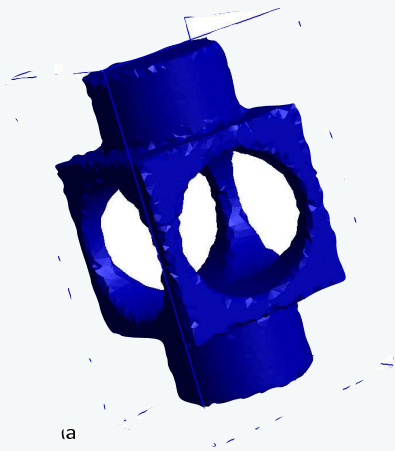


Examples

- multiple level sets



- single (left) versus multiple (right)

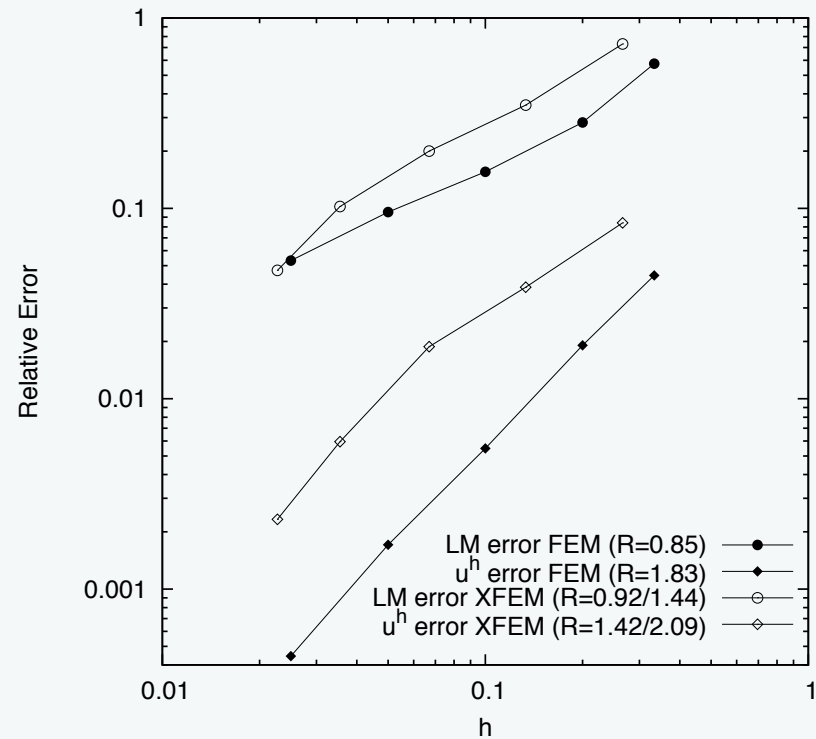
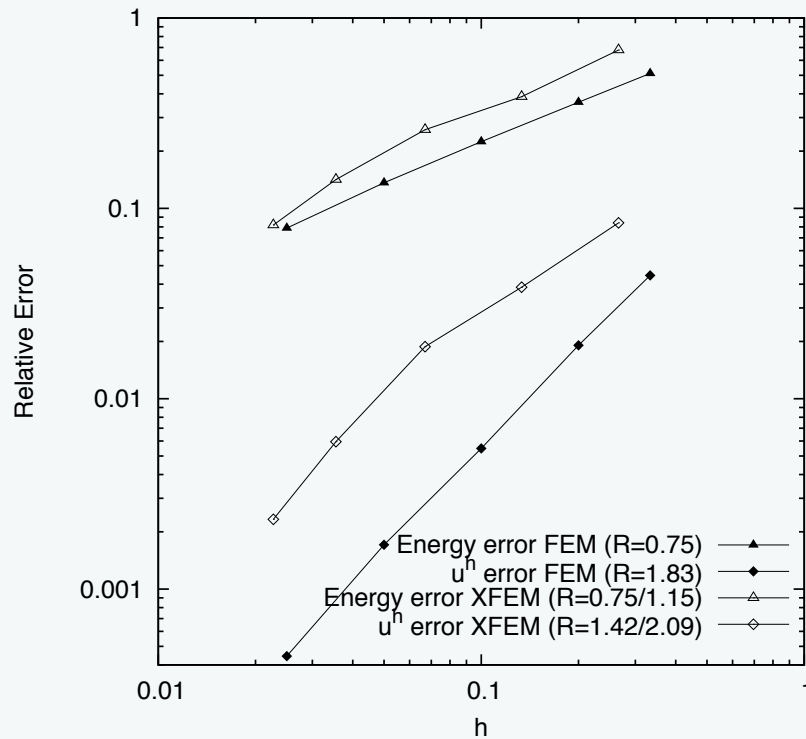
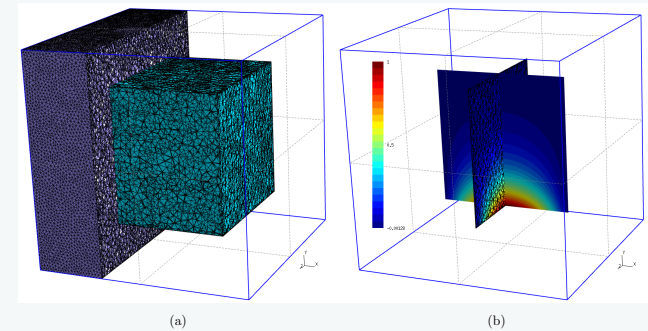


- Laplace equation on a cube

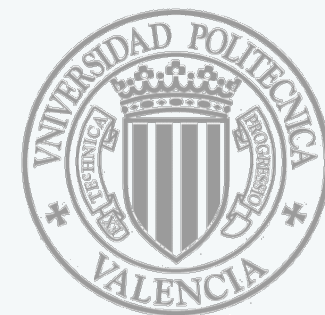
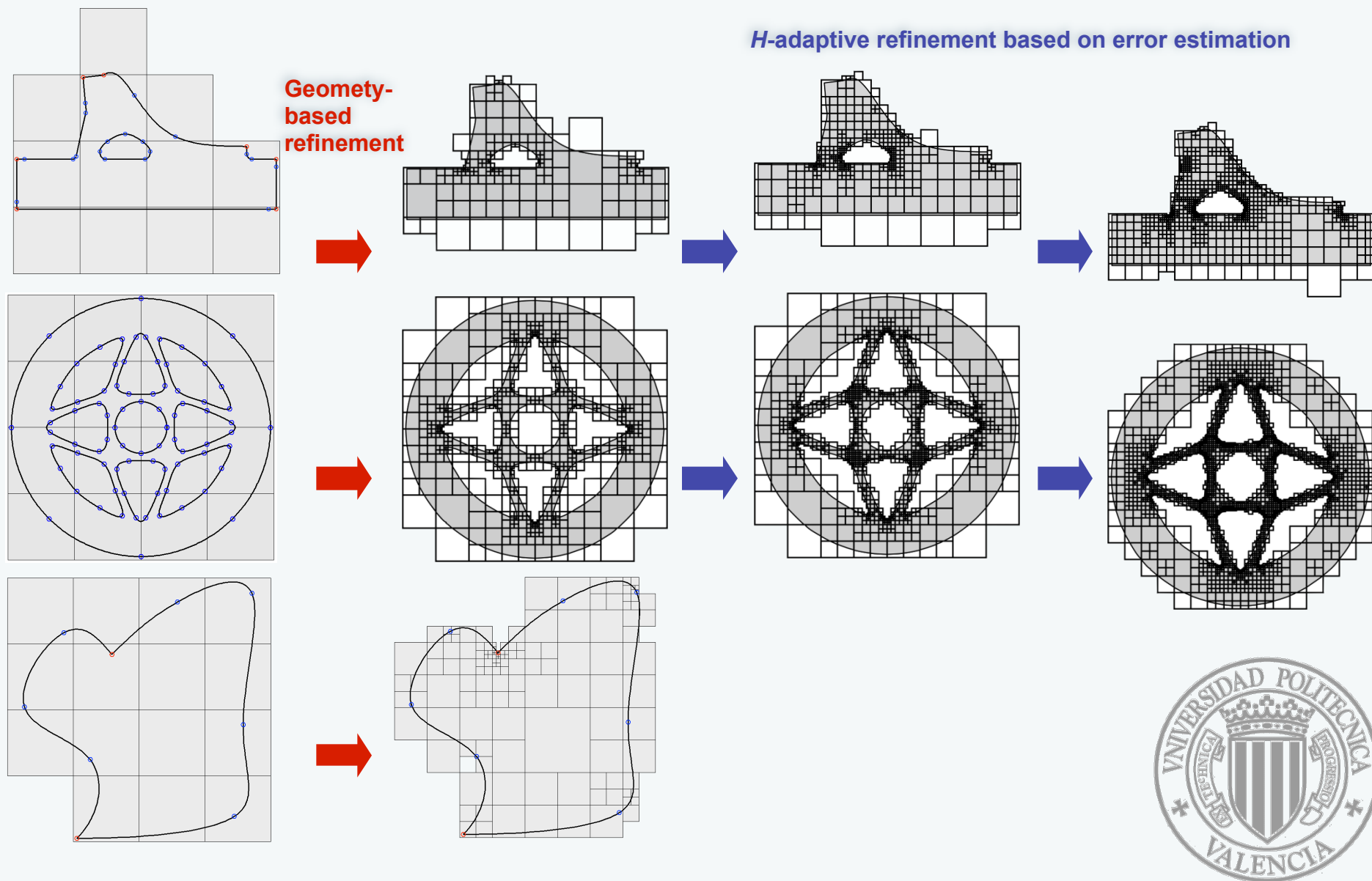
- convergence rates

➡ optimal

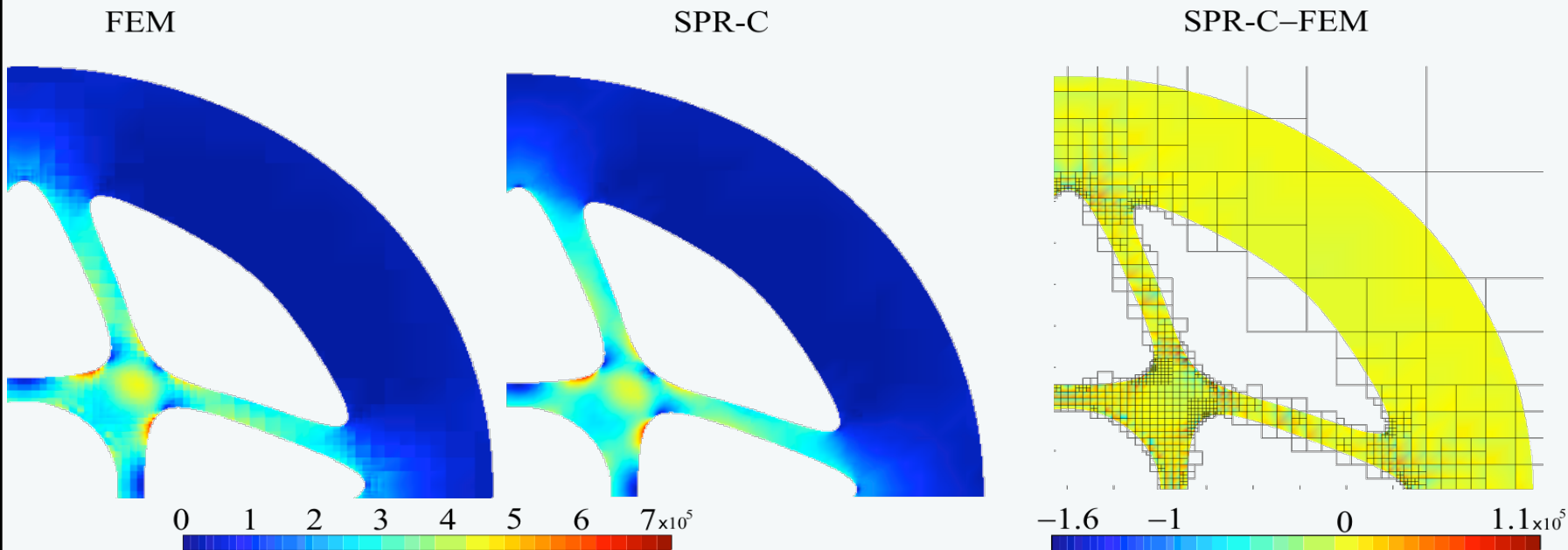
➡ requires proper Lagrange multiplier space to eradicate spurious oscillations



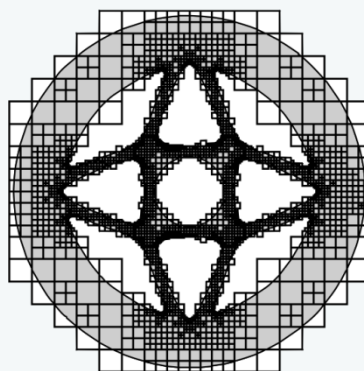
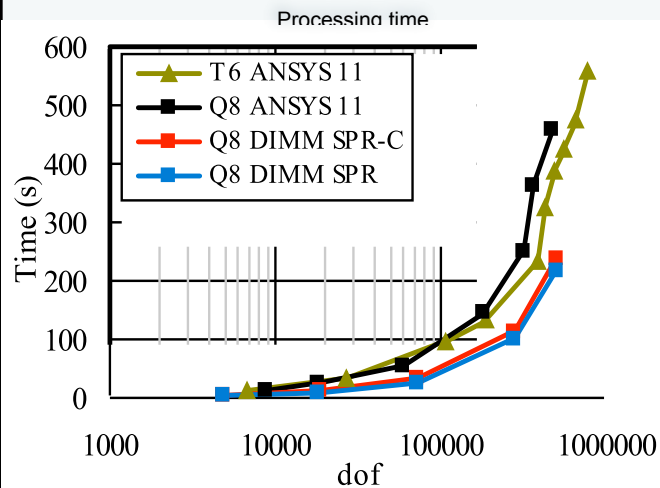
Pixel/Voxel-based FEA on Cartesian grids (Valencia)



Pixel/Voxel-based FEA on Cartesian grids (Valencia)



Quad8 uniform refinement

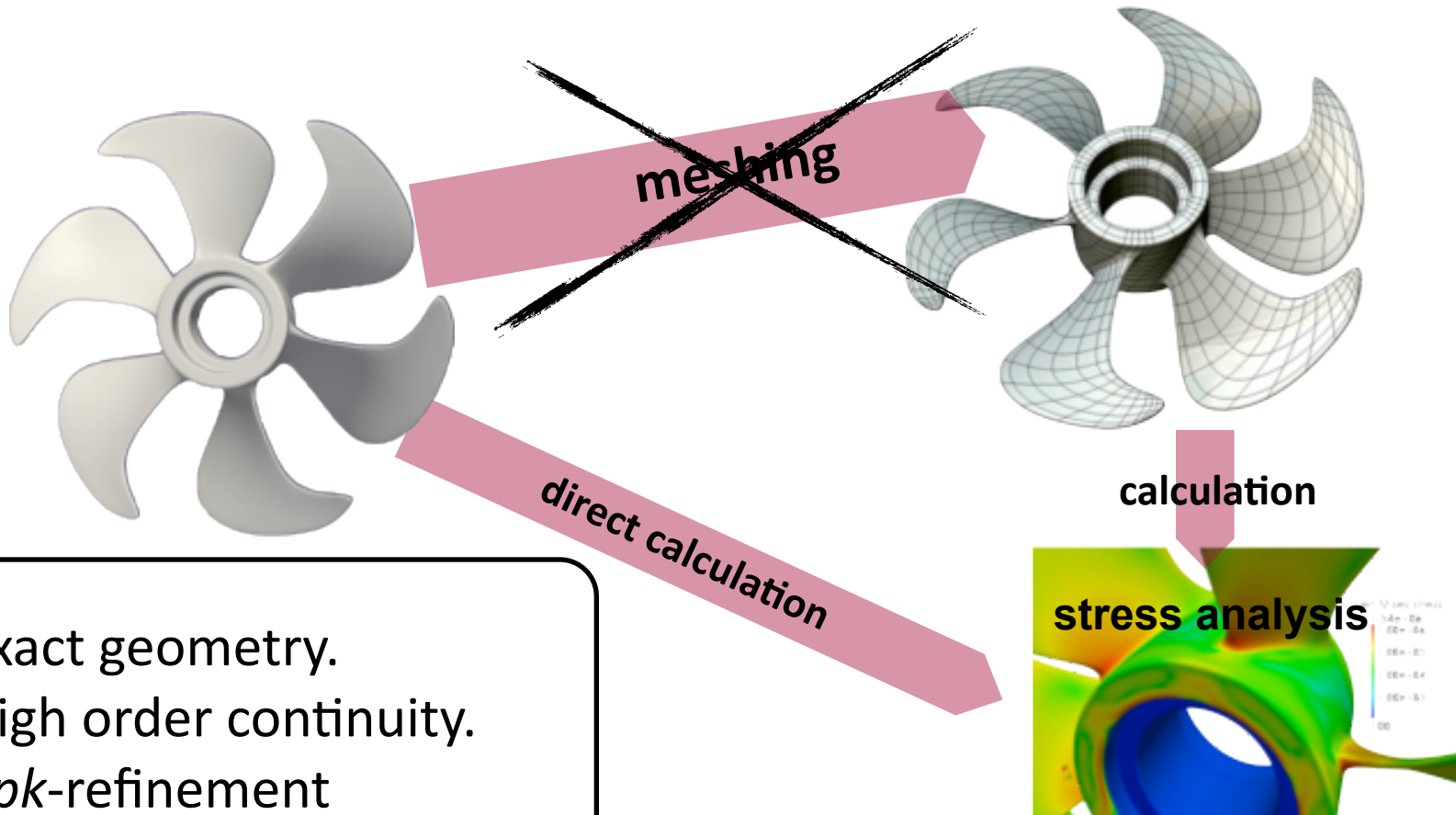


Paradigm 2 : IGA

Couple Geometry and Approximation

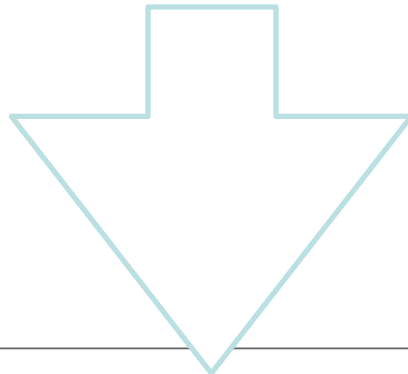


Approximate the unknown fields with the same basis functions (NURBS, T-splines ...) as that used to generate the CAD model



1. Generate a **volume** discretization using the **surface** geometry only?
2. Realistic solids can in general not be represented by only one volume (patch) and multiple **patches** must be **glued** together to avoid “leaks” (Nitsche, T-splines, PHT-splines, RL/LR-splines)
3. Refinement must be done everywhere in the domain (T, PHT... splines)

3 KEY QUESTIONS FOR IGA



Isogeometric Analysis with BEM



1. IGABEM with NURBS for 2D elastic problems (Simpson, *et al.* CMAME, 2011).
2. IGABEM with T-splines for 3D elastic problems (Scott, *et al.* CMAME, 2012).
3. IGABEM with T-splines for 3D acoustic problems (Simpson, *et al.* 2013 - MAFELAP2013 TH1515).

Difficulties in dealing with nonlinear problems and non-homogeneous materials.

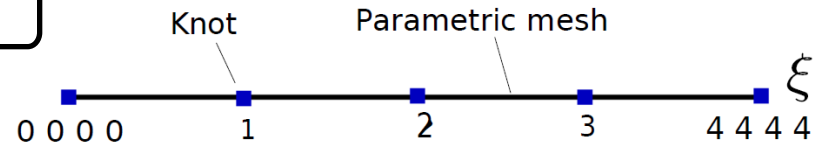
Non-uniform rational B-splines

Knot vector

a non-decreasing set of coordinates in the parametric space.

$$\Xi = \{\xi_1, \xi_2, \dots, \xi_{n+p+1}\}$$

B-spline basis function

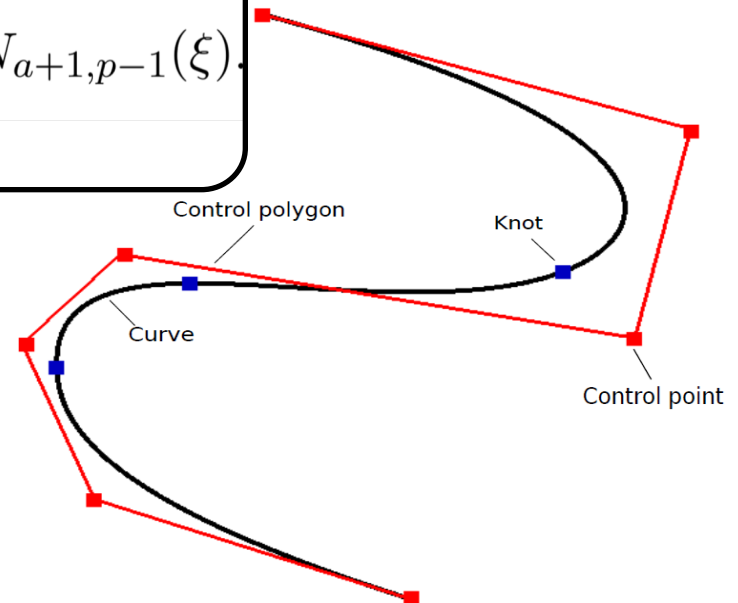


$$N_{a,0}(\xi) = \begin{cases} 1, & \text{if } \xi_a \leq \xi < \xi_{a+1} \\ 0, & \text{otherwise.} \end{cases}$$

$$N_{a,p}(\xi) = \frac{\xi - \xi_a}{\xi_{a+p} - \xi_a} N_{a,p-1}(\xi) + \frac{\xi_{a+p+1} - \xi}{\xi_{a+p+1} - \xi_{a+1}} N_{a+1,p-1}(\xi)$$

NURBS basis function

$$R_{a,p}(\xi) = \frac{N_{a,p}(\xi)w_a}{W(\xi)} = \frac{N_{a,p}(\xi)w_a}{\sum_{\hat{a}=1}^n N_{\hat{a},p}w_{\hat{a}}},$$





- Partition of Unity

$$\sum_{i=1}^n R_{i,p}(\xi) = 1$$

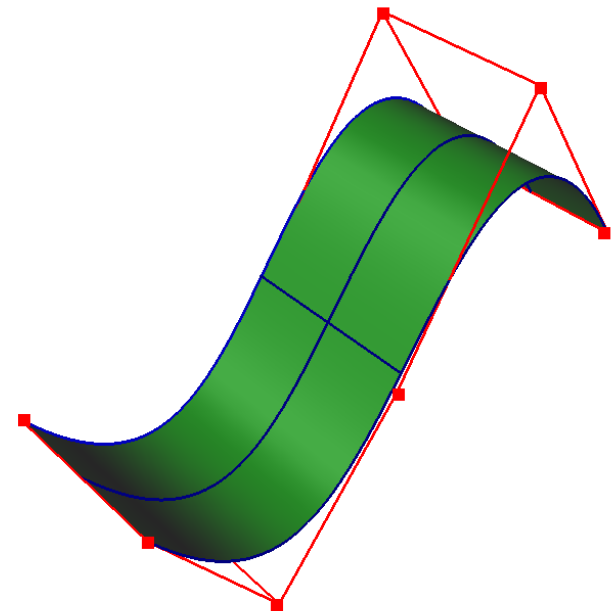
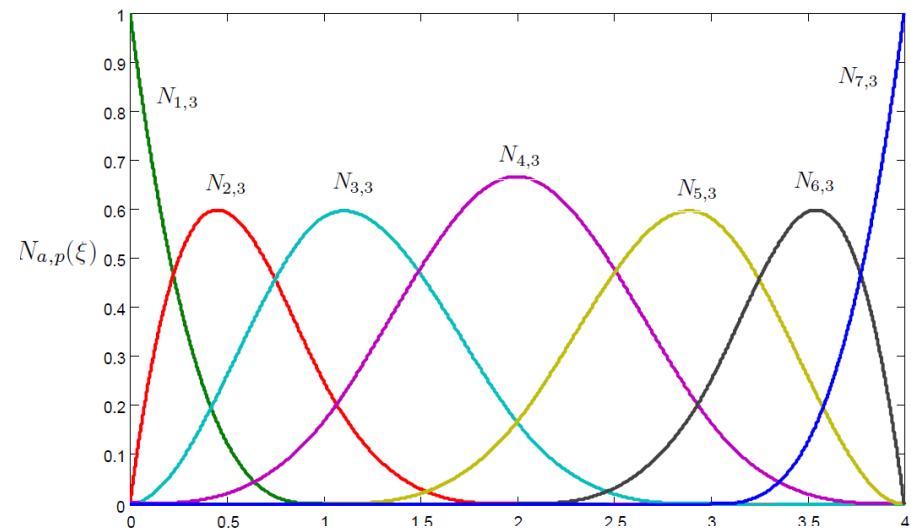
- Non-negative

- $p-1$ continuous derivatives

- Tensor product property

$$S(\xi, \eta) = \sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) \mathbf{B}_{i,j}$$

$$\sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) = \left(\sum_{i=1}^n R_{i,p}^1(\xi) \right) \left(\sum_{j=1}^m R_{j,q}^2(\eta) \right)$$



NURBS to T-splines



(NURBS geometry)



(T-splines geometry)

NURBS

- No watertight geometry
- No local refinement scheme

T-splines

- Local knot vector (as Point-based splines)
- Global topology

Y. Bazilevs, V.M. Calo, J.A. Cottrell, J.A. Evans, T.J.R. Hughes, S. Lipton, M.A. Scott, and T.W. Sederberg. Isogeometric analysis using T-splines. CMAME, 199(5-8):229–263, 2010.

IGABEM formulation

Regularised form of boundary integral equation for 2D linear elasticity

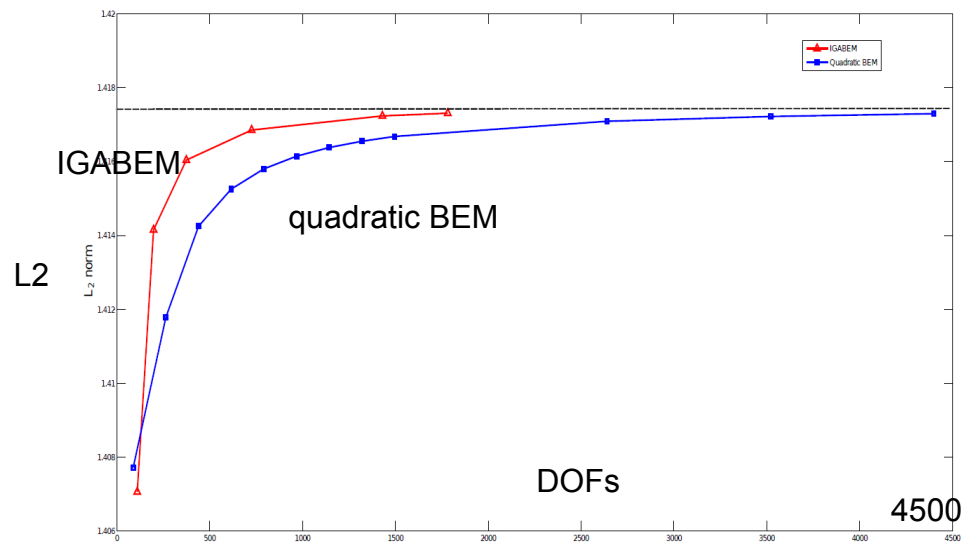
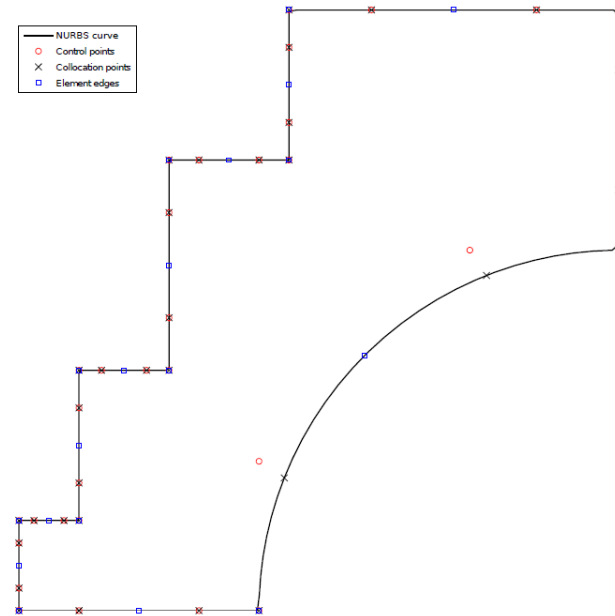
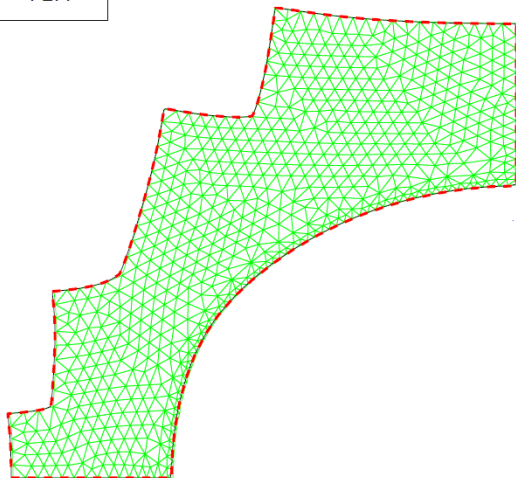
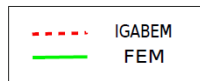
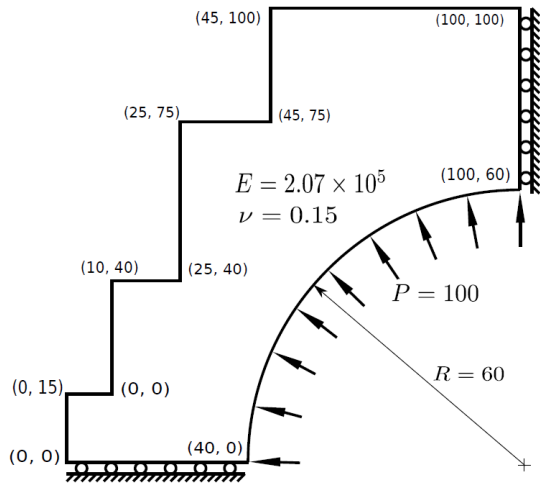
$$\int_{\Gamma} \mathbf{T}(\mathbf{s}, \mathbf{x}) [\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{s})] d\Gamma(\mathbf{x}) = \int_{\Gamma} \mathbf{U}(\mathbf{s}, \mathbf{x}) \mathbf{t}(\mathbf{x}) d\Gamma(\mathbf{x})$$

where \mathbf{x} and \mathbf{s} are field point and source point respectively, \mathbf{u} and \mathbf{t} are displacement and traction around the boundary, \mathbf{T} and \mathbf{U} are fundamental solutions.

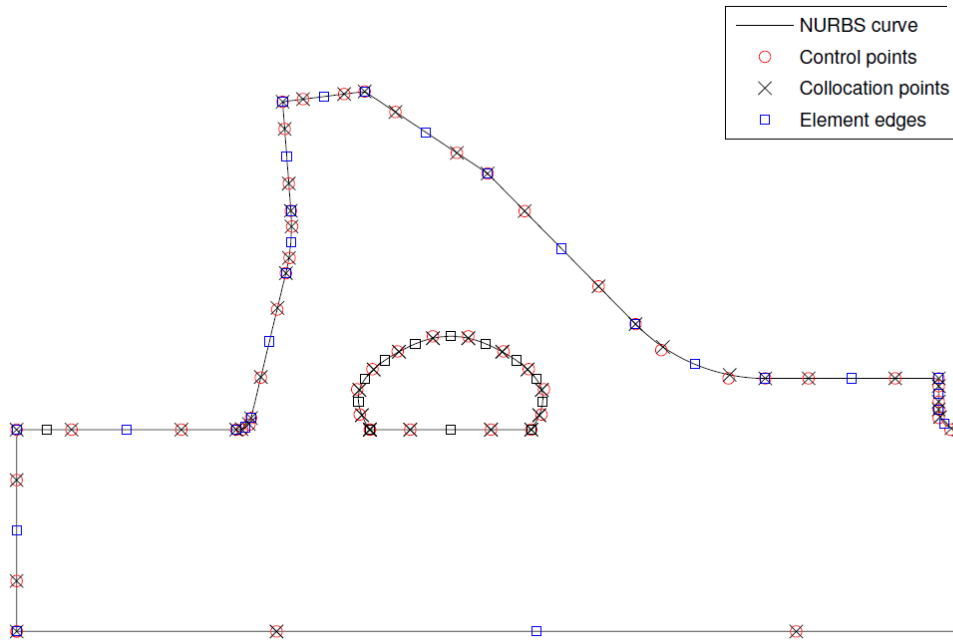
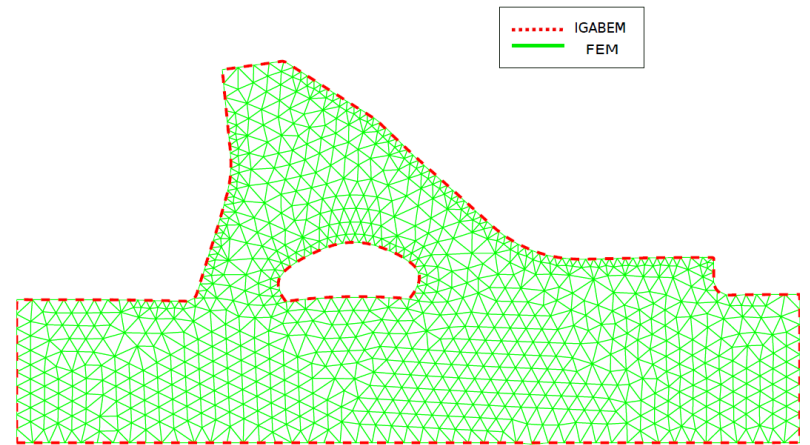
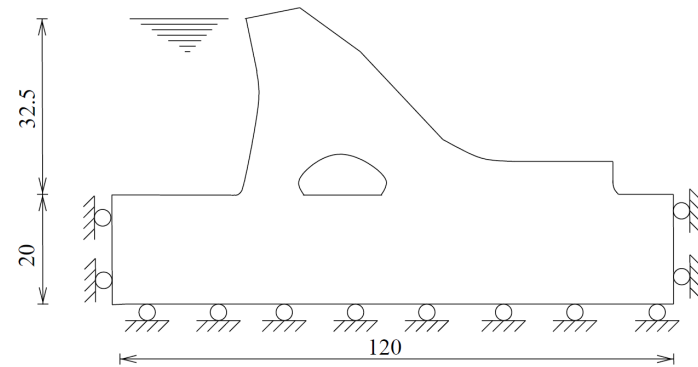
Discretise the geometry and solution field using NURBS

$$\begin{aligned} \mathbf{x} &= \sum_{A=1}^{n_A} N_A(\xi) \mathbf{B}_A = N_A(\xi) \mathbf{B}_A \\ \mathbf{u} &= \sum_{A=1}^{n_A} N_A(\xi) \mathbf{u}_A = N_A(\xi) \mathbf{u}_A \\ \mathbf{t} &= \sum_{B=1}^{n_B} N_B(\xi) \mathbf{t}_B = N_B(\xi) \mathbf{t}_B \end{aligned}$$

Nuclear reactor



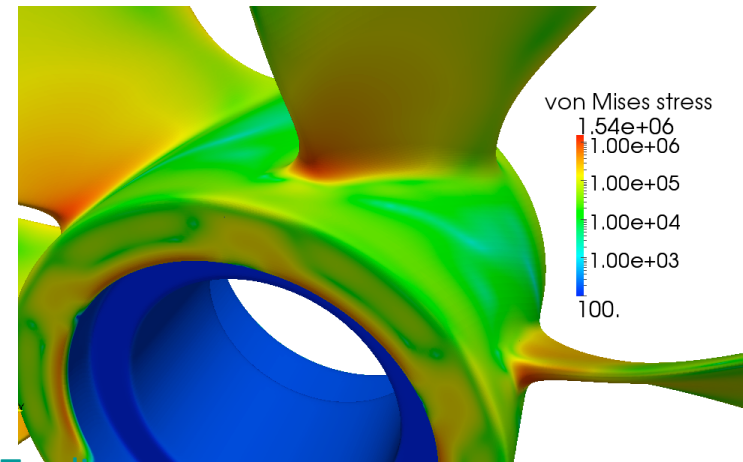
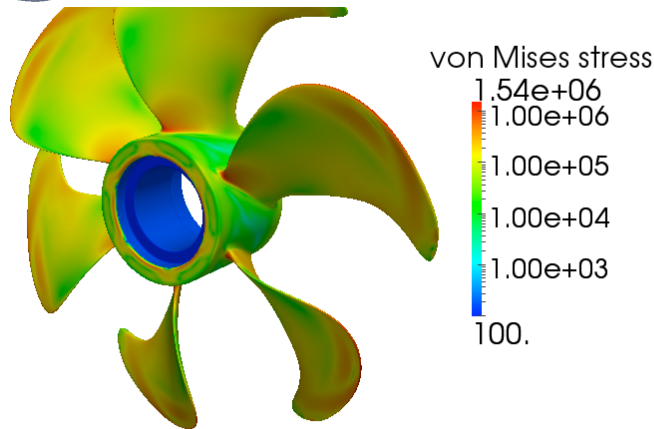
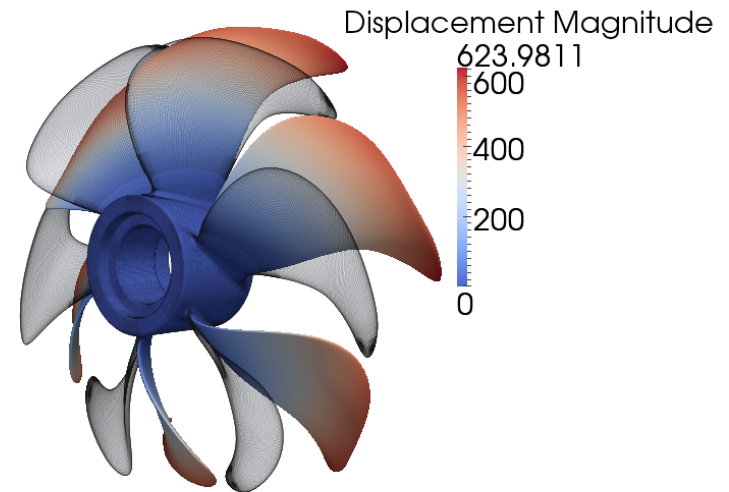
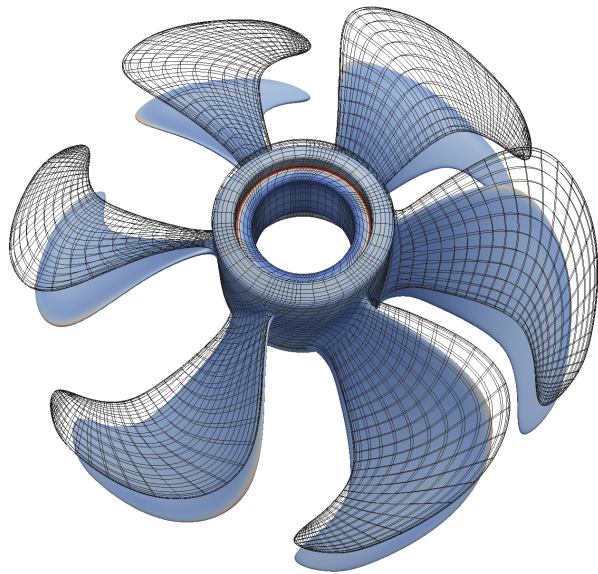
Dam



Stress analysis without meshing: isogeometric boundary-element method

ICE Proceeding, 2013, H Lian, RN Simpson, SPA Bordas

Propeller: NURBS would require several patches - single patch T-splines



Isogeometric boundary element analysis using unstructured T-splines

MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg
CMAME, 2013.

Part II. Some recent advances in enriched FEM



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INSIST

Handling discontinuities in isogeometric formulations

Faculty of Sciences,
Technology
and Communication

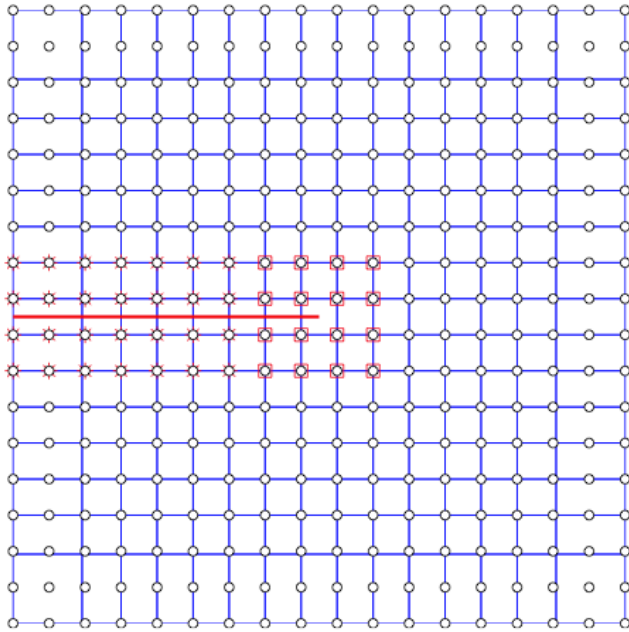
erc

with Nguyen Vinh Phu, Marie Curie Fellow

68

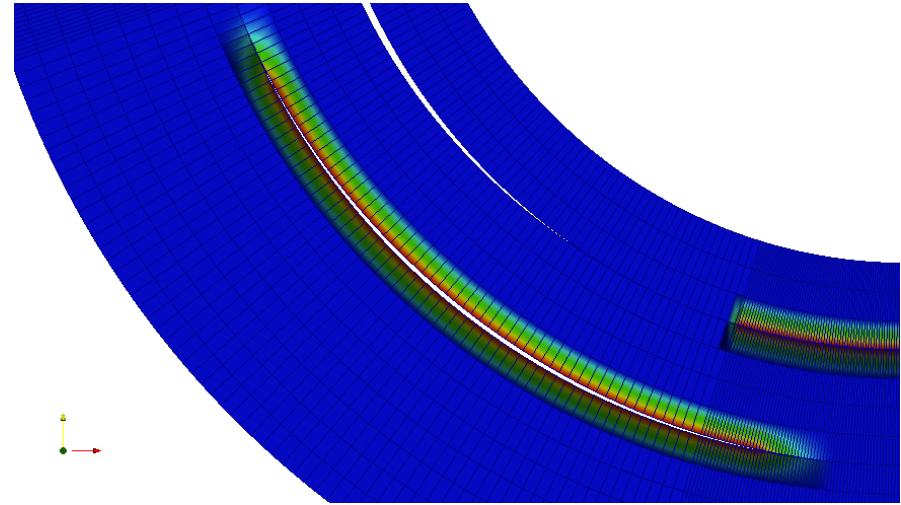


PUM enriched methods



- IGA: link to CAD and accurate stress fields
- XFEM: no remeshing

Mesh conforming methods



- IGA: link to CAD and accurate stress fields
- Apps: delamination



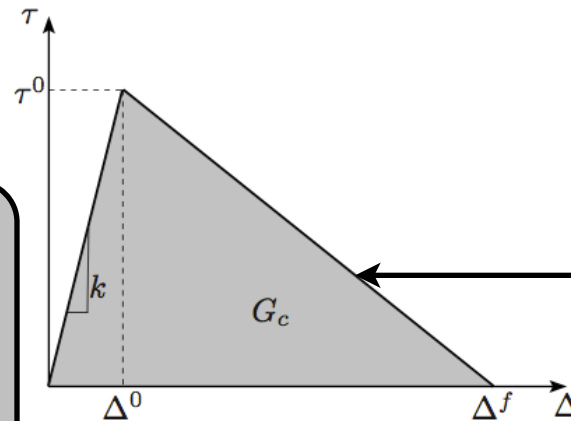
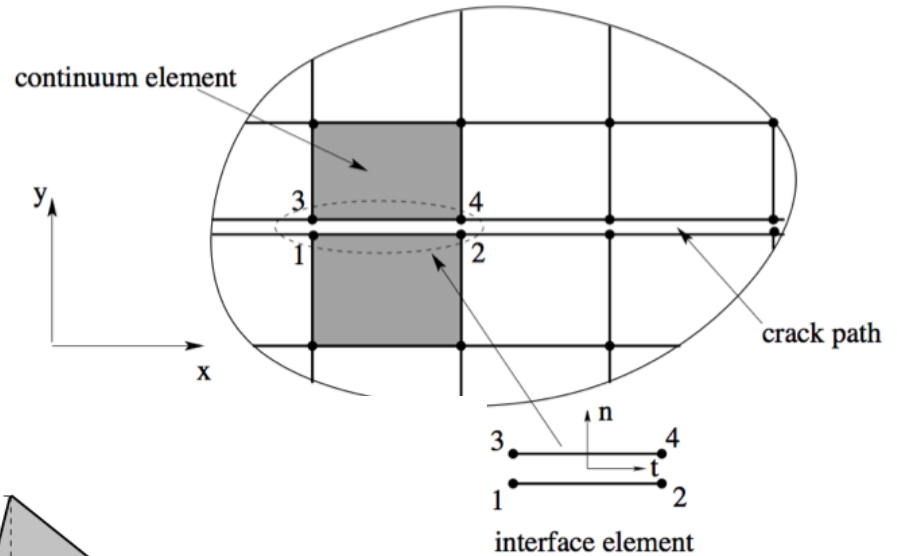
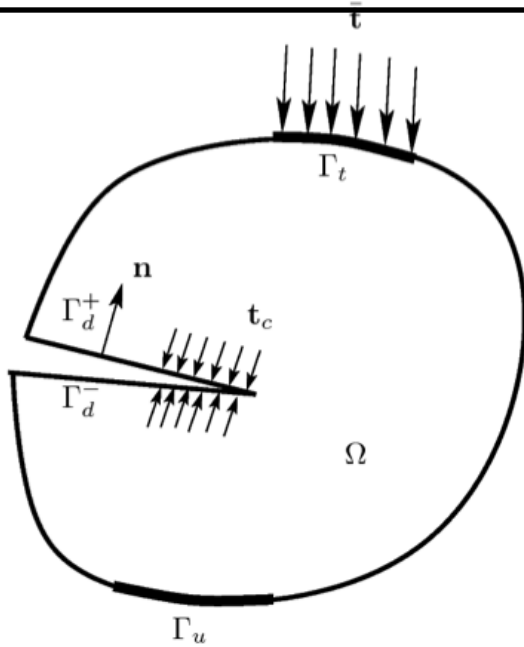
$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} R_I(\mathbf{x}) \mathbf{u}_I + \sum_{J \in \mathcal{S}^c} R_J(\mathbf{x}) \Phi(\mathbf{x}) \mathbf{a}_J$$

NURBS basis functions

enrichment functions

1. E. De Luycker, D. J. Benson, T. Belytschko, Y. Bazilevs, and M. C. Hsu. X-FEM in isogeometric analysis for linear fracture mechanics. IJNME, 87(6):541–565, 2011.
2. S. S. Ghorashi, N. Valizadeh, and S. Mohammadi. Extended isogeometric analysis for simulation of stationary and propagating cracks. IJNME, 89(9): 1069–1101, 2012.
3. D. J. Benson, Y. Bazilevs, E. De Luycker, M.-C. Hsu, M. Scott, T. J. R. Hughes, and T. Belytschko. A generalized finite element formulation for arbitrary basis functions: From isogeometric analysis to XFEM. IJNME, 83(6):765–785, 2010.
4. A. Tambat and G. Subbarayan. Isogeometric enriched field approximations. CMAME, 245–246:1 – 21, 2012.

Delamination analysis with cohesive elements (standard approach)

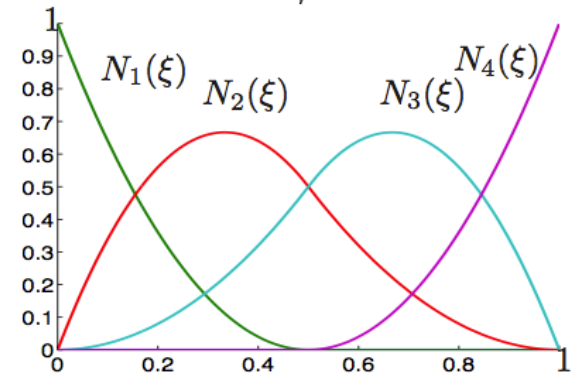
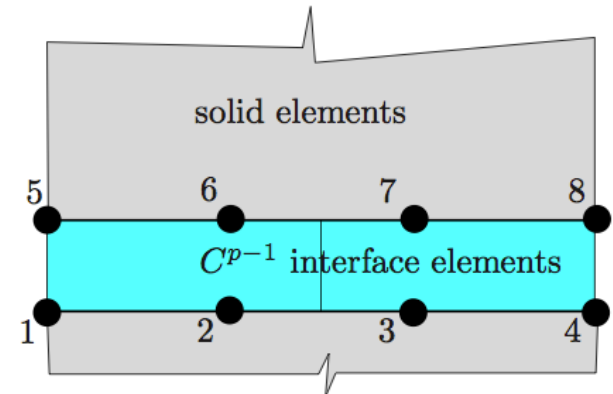
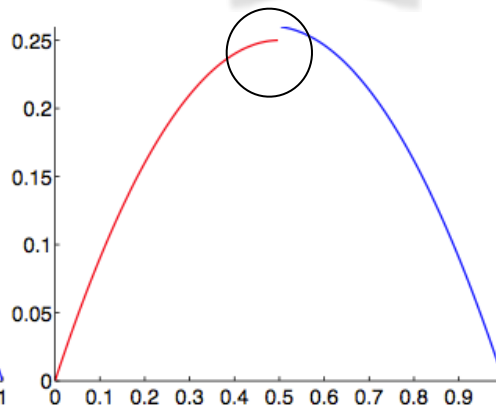
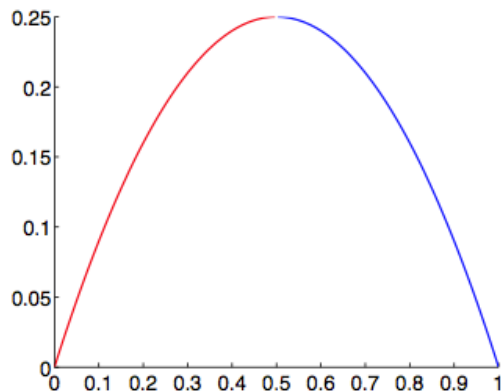
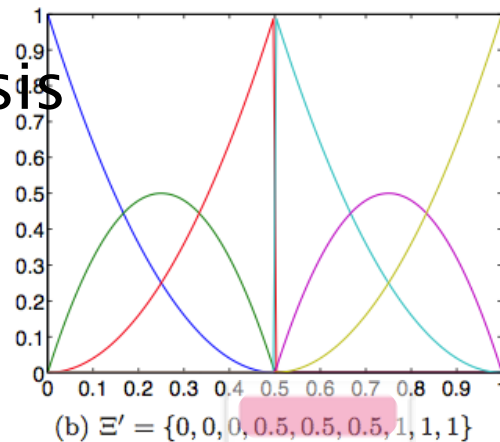
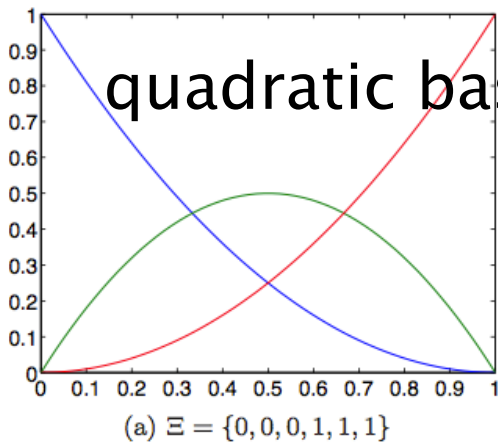


- No link to CAD
- Long preprocessing
- Refined meshes

$$\int_{\Omega} \delta \mathbf{u} \cdot \mathbf{b} d\Omega + \int_{\Gamma_t} \delta \mathbf{u} \cdot \bar{\mathbf{t}} d\Gamma_t = \int_{\Omega} \delta \boldsymbol{\epsilon} : \boldsymbol{\sigma}(\mathbf{u}) d\Omega + \int_{\Gamma_d} \delta [\![\mathbf{u}]\!] \cdot \mathbf{t}^c([\![\mathbf{u}]\!]) d\Gamma_d$$

Isogeometric cohesive elements

quadratic basis

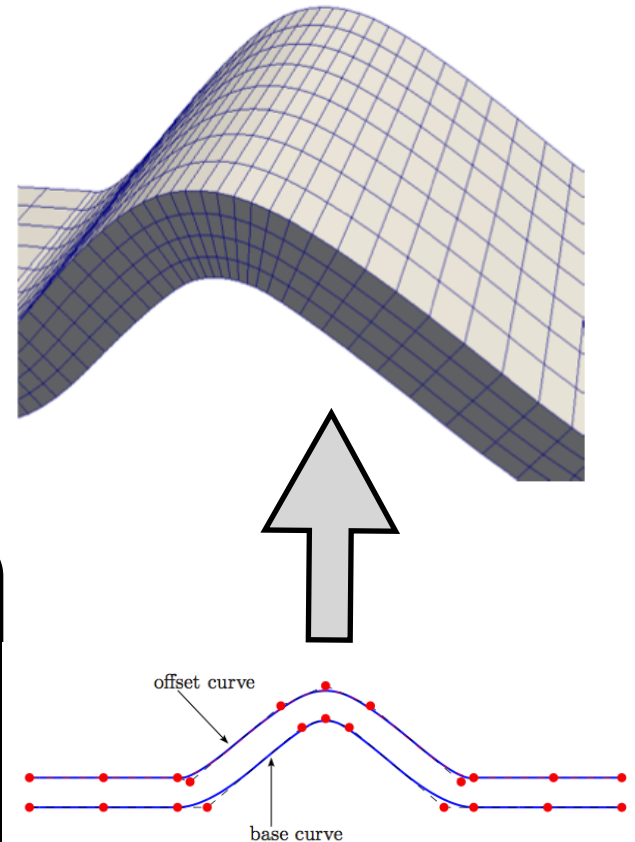


Knot insertion

1. C. V. Verhoosel, M. A. Scott, R. de Borst, and T. J. R. Hughes. An isogeometric approach to cohesive zone modeling. *IJNME*, 87(15):336–360, 2011.
2. V.P. Nguyen, P. Kerfriden, S. Bordas. Isogeometric cohesive elements for two and three dimensional composite delamination analysis, 2013, Arxiv.

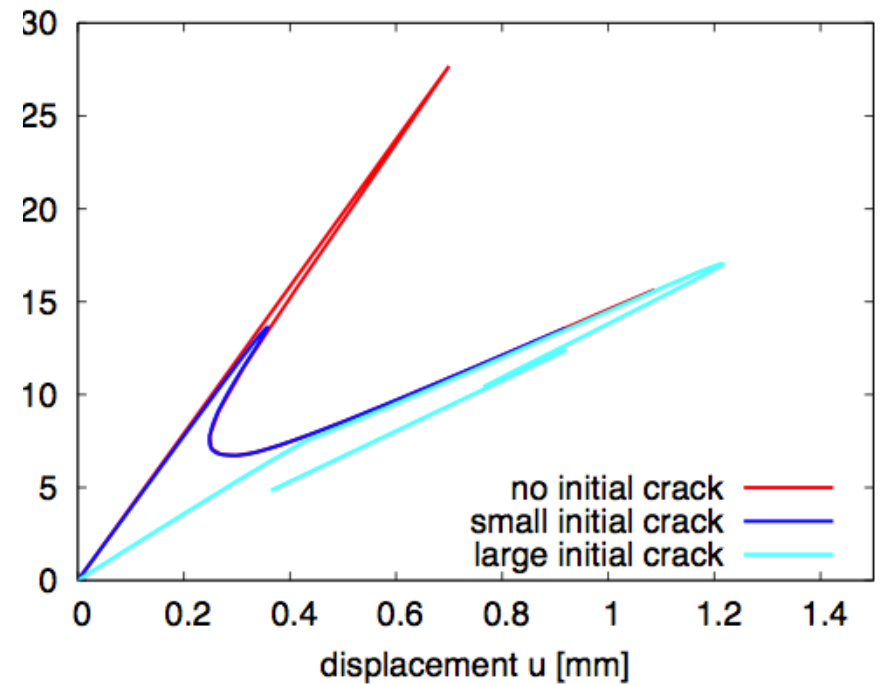
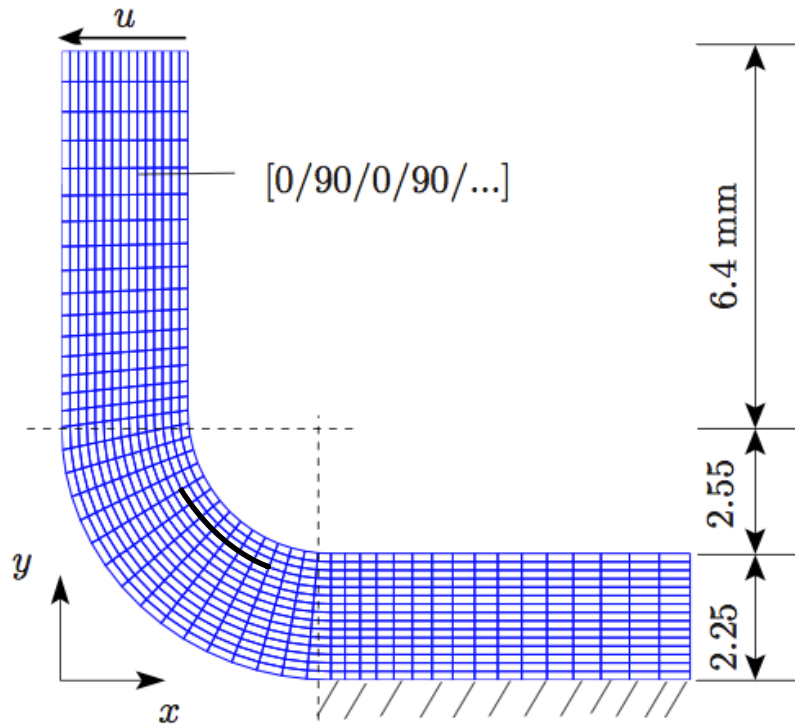
Isogeometric cohesive elements: advantages

- Direct link to CAD
 - Exact geometry
 - Fast/straightforward generation of interface elements
 - Accurate stress field
 - Computationally cheaper
-
- 2D Mixed mode bending test (MMB)
 - 2 x 70 quartic-linear B-spline elements
 - Run time on a laptop 4GBi7: 6 s
 - Energy arc-length control

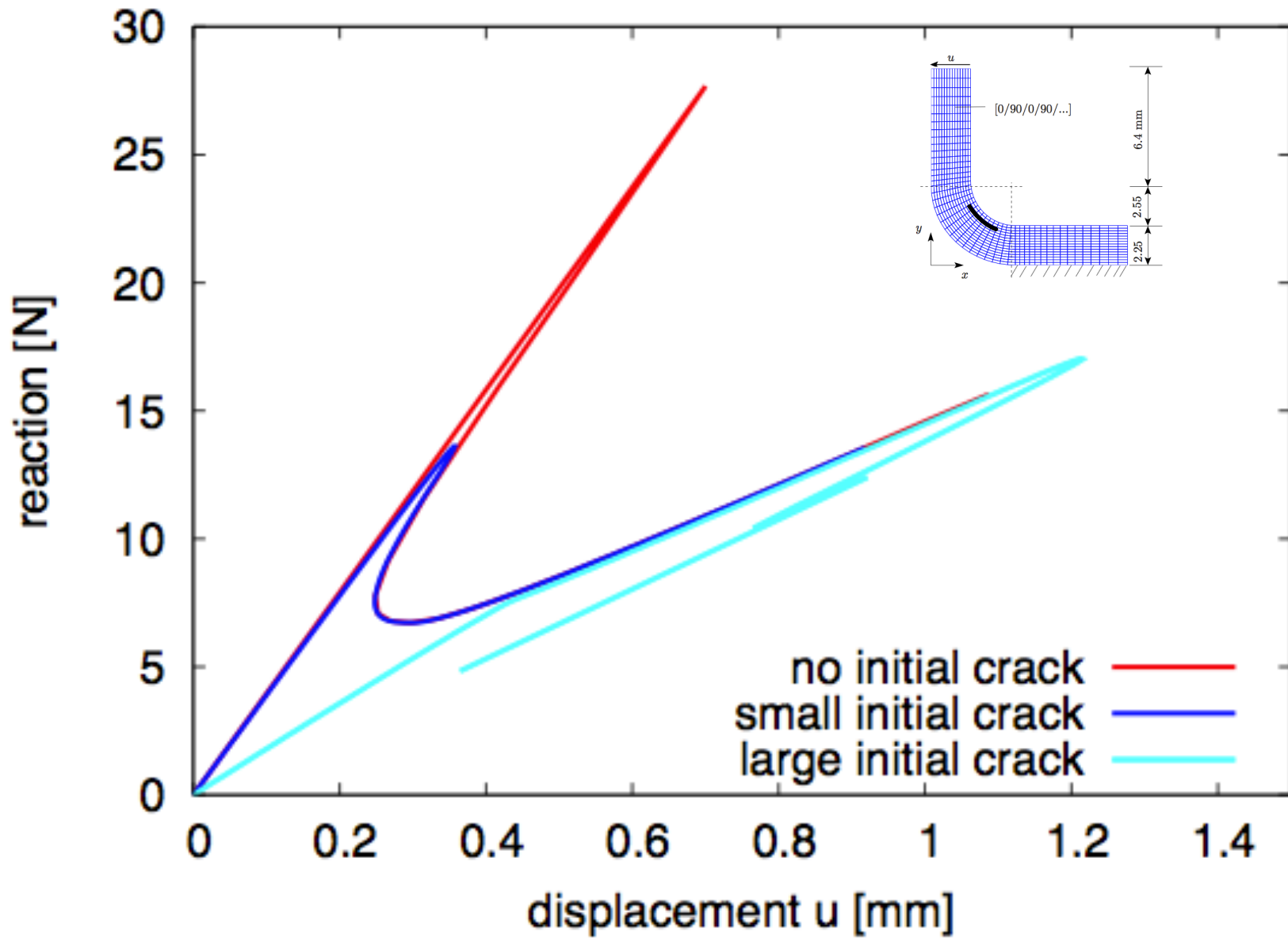


V. P. Nguyen and H. Nguyen-Xuan. High-order B-splines based finite elements for delamination analysis of laminated composites. *Composite Structures*, 102:261–275, 2013.

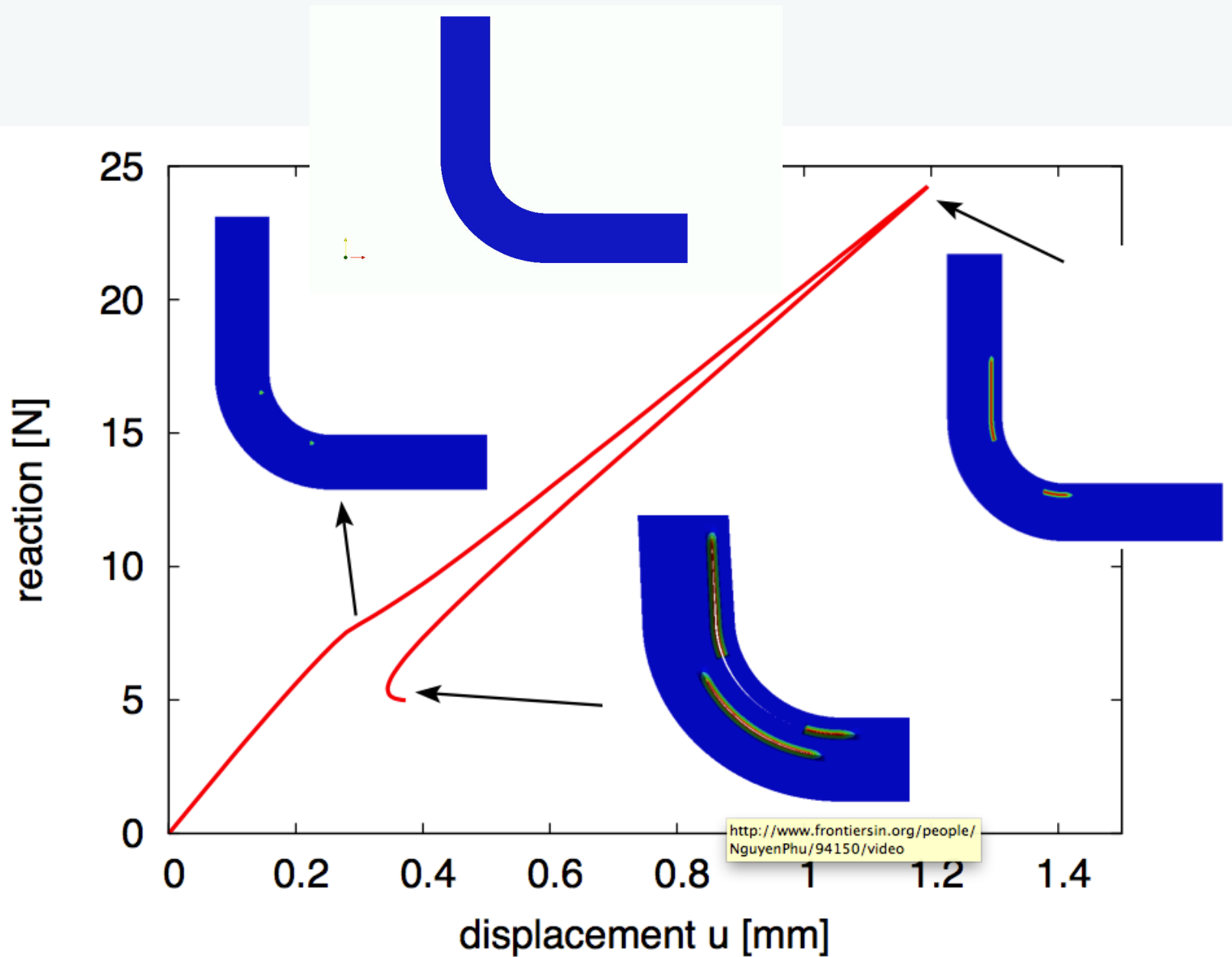
Isogeometric cohesive elements: 2D example



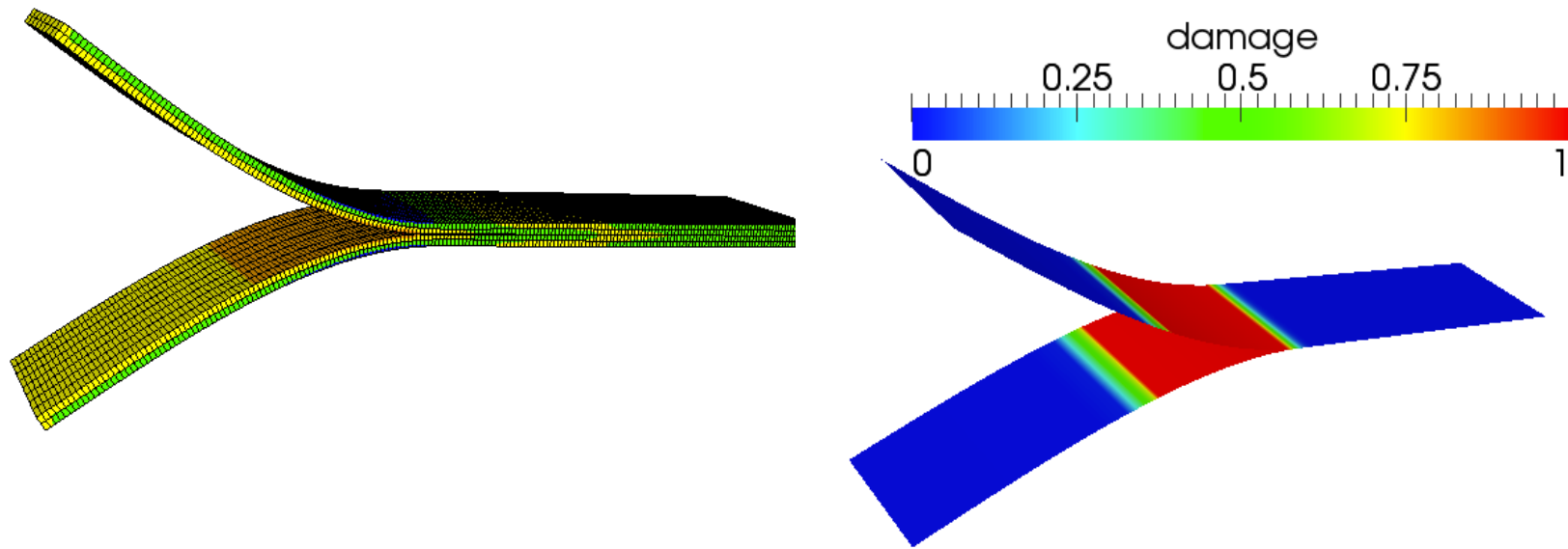
- Exact geometry by NURBS + direct link to CAD
- It is straightforward to vary
 - (1) the number of plies and
 - (2) # of interface elements:
- Suitable for parameter studies/design
- Solver: energy-based arc-length method (Gutierrez, 2007)



Isogeometric cohesive elements: 2D example

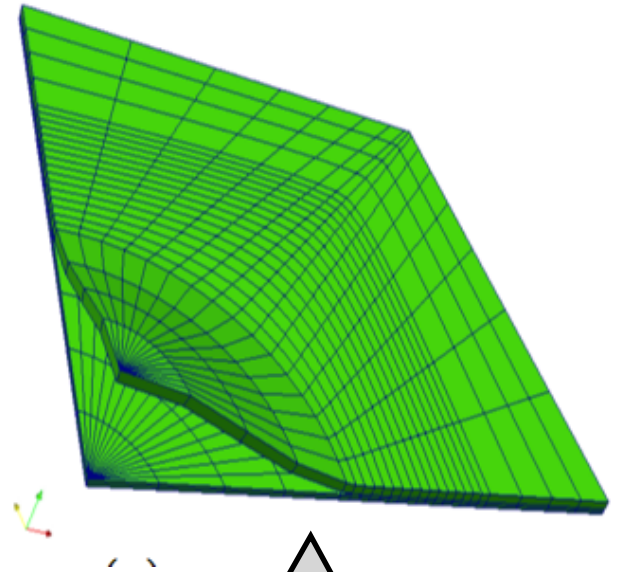
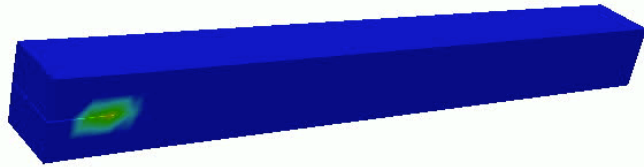


Isogeometric cohesive elements: 3D example with shells

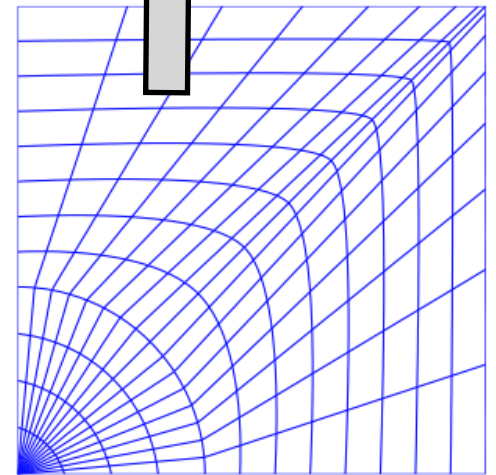
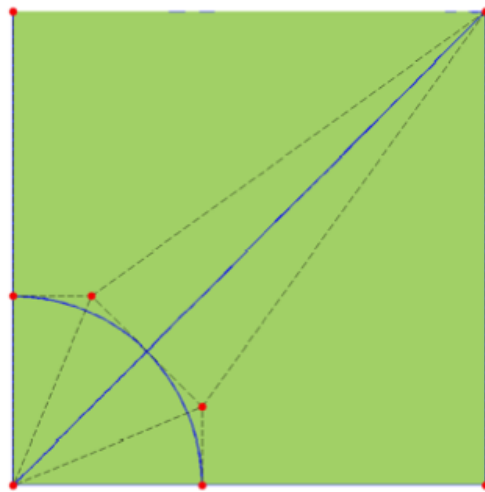


- Rotation free B-splines shell elements (Kiendl et al. CMAME)
- Two shells, one for each lamina
- Bivariate B-splines cohesive interface elements in between

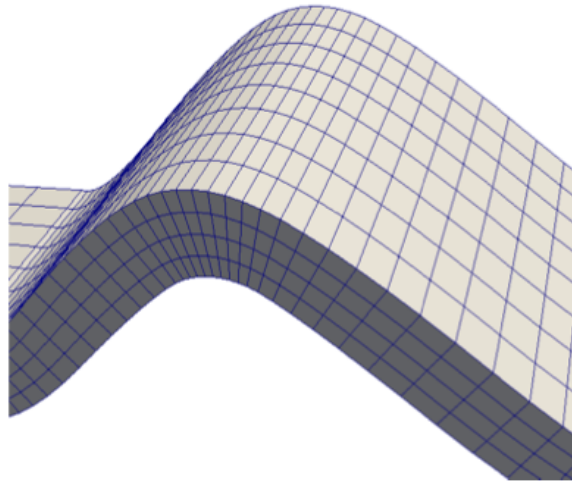
Isogeometric cohesive elements: 3D examples



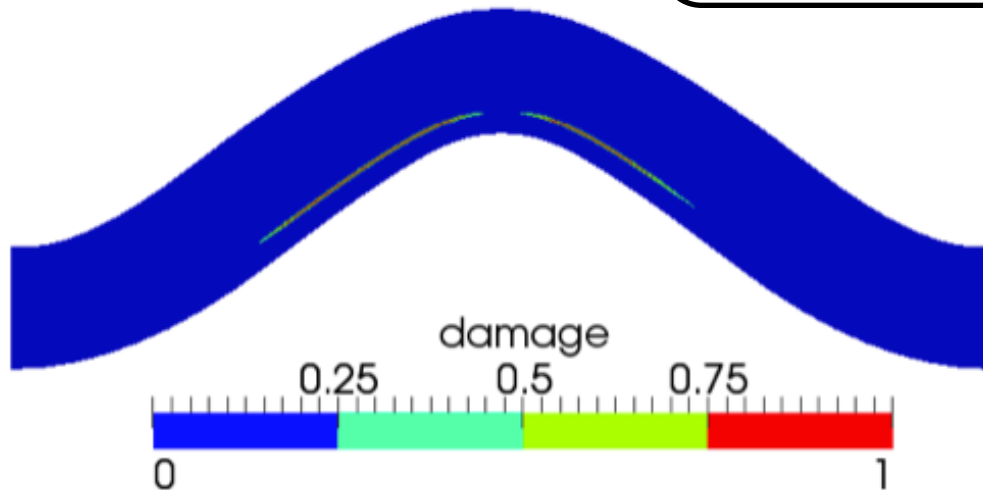
- cohesive elements for 3D meshes the same as 2D
- large deformations



Isogeometric cohesive elements



- singly curved thick-wall laminates
- geometry/displacements: NURBS
- trivariate NURBS from NURBS surface(*)
- cohesive surface interface elements



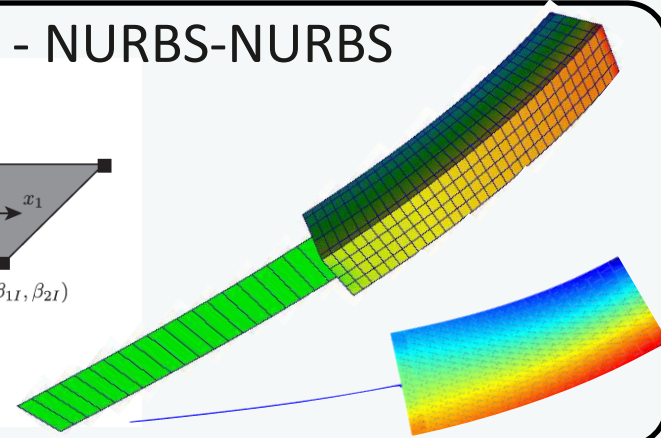
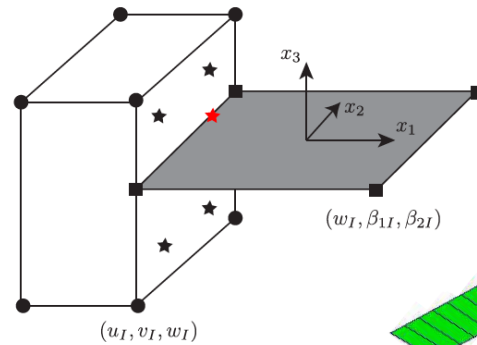
(*)V. P. Nguyen, P. Kerfriden, S.P.A. Bordas, and T. Rabczuk. An integrated design-analysis framework for three dimensional composite panels. Computer Aided Design, 2013. submitted.

Future work: model selection (continuum, plate, beam, shell?)

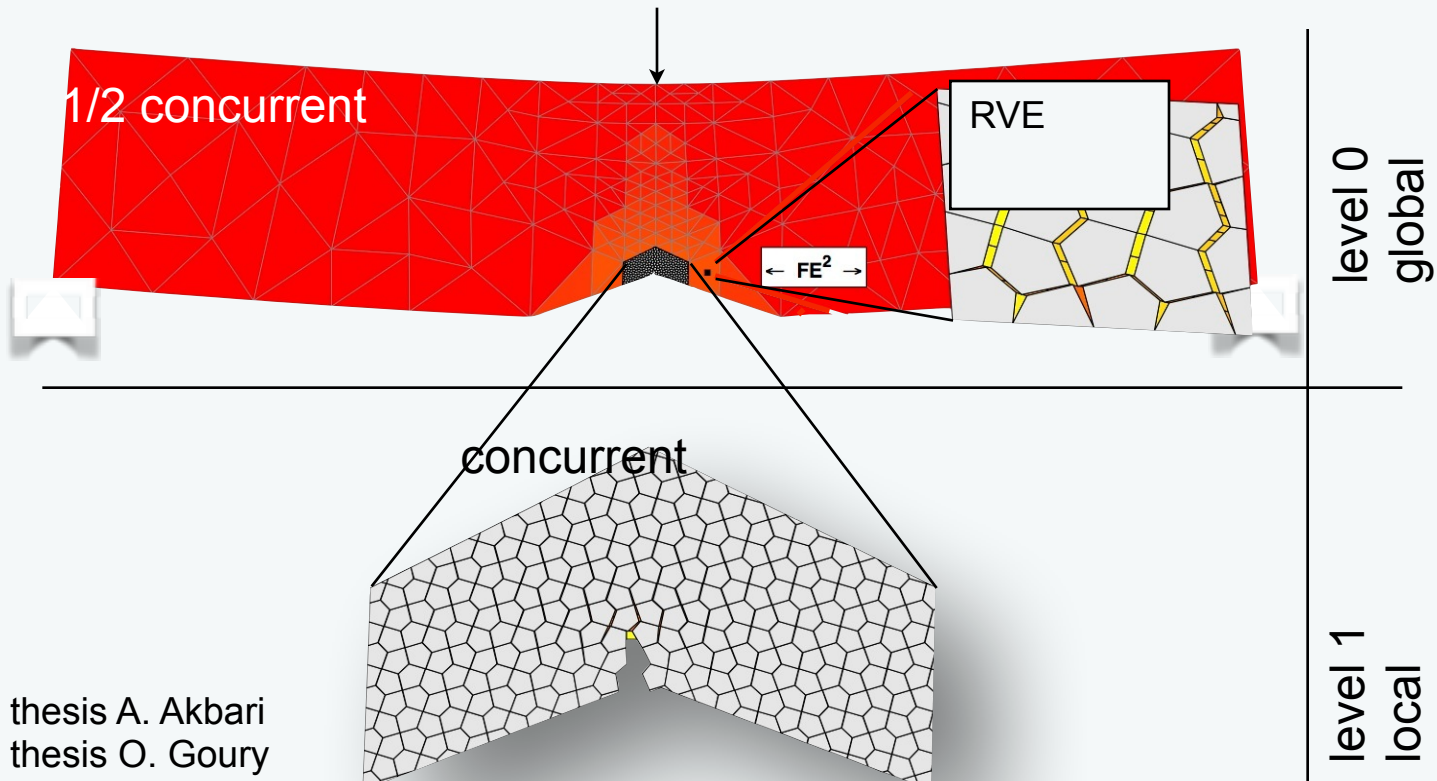
Model selection

- Model with shells
- Identify “hot spots” - dual
- Couple with continuum
- Coarse-grain

• Nitsche coupling - NURBS-NURBS



load



Part III. Application to multi-crack propagation

with Danas Sutula, President Scholar



Faculty of Sciences,
Technology
and Communication

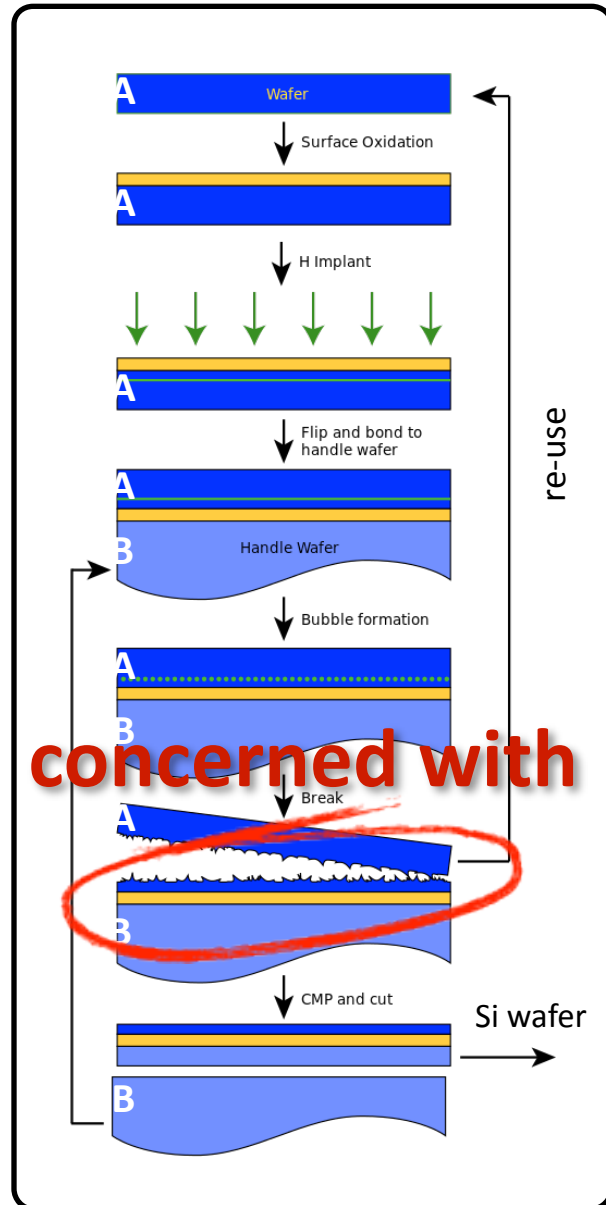
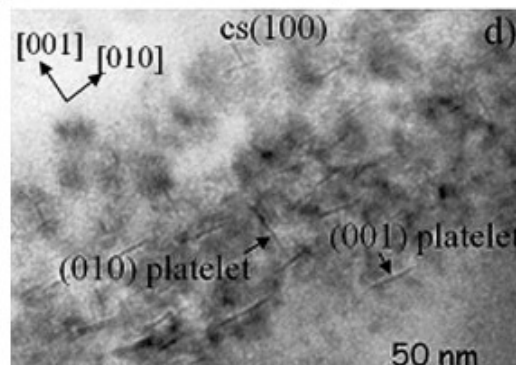
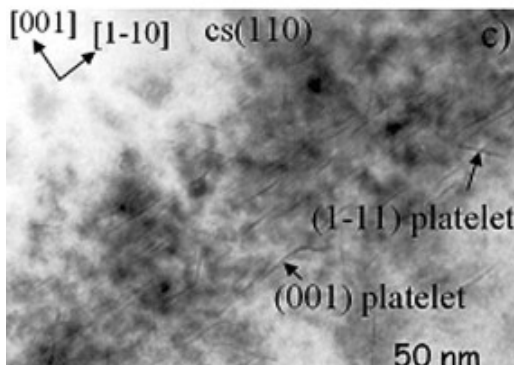


Numerical Modeling of SOI Wafer Splitting



Manufacturing process: *SmartCut*TM

- H^+ ionization of a thin surface of Si
- Bonding to a handle-wafer (stiffener)
- High temperature thermal annealing
- Nucleation and growth of cavities filled with H_2
- Pressure driven micro crack growth
- Coalescence and post-split fracture roughness



Determine:

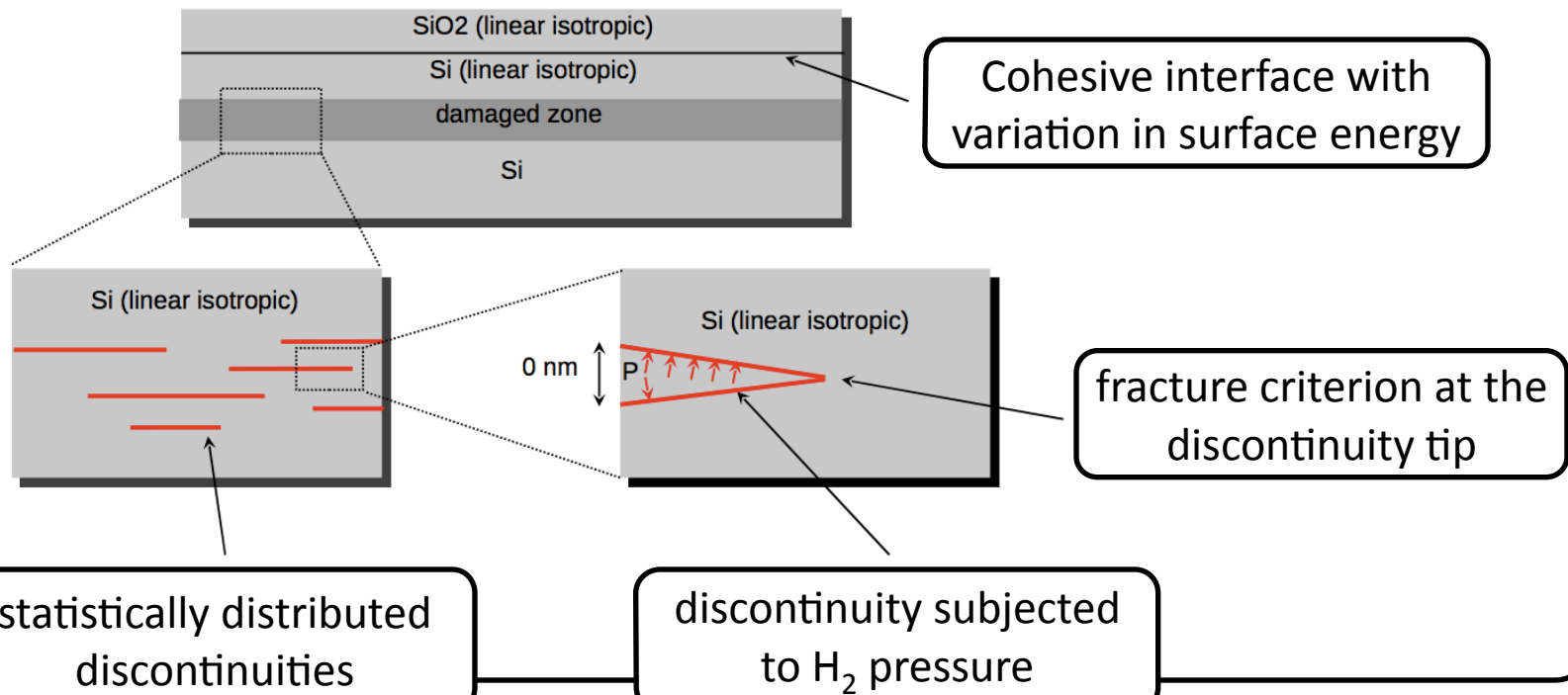
- micro crack nucleation points and direction
- multiple crack paths until coalescence
- time to complete fracture
- final surface roughness

Modeling cavities by zero thickness surfaces

- discontinuities in the displacement field

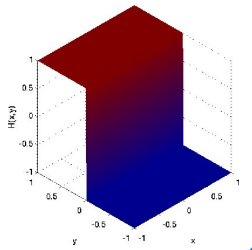
Linear elastic fracture mechanics (LEFM)

- infinite stress at crack tip, i.e. *singularity*



Approximation function:

$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4 f_{\alpha}(\mathbf{x}) \mathbf{b}^{K\alpha}}_{\text{singular tip enrichment}}$$

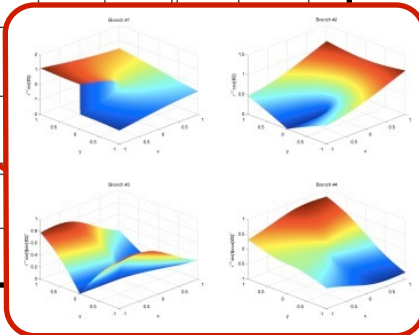


$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

$$\{f_{\alpha}(r, \theta), \alpha = 1, 4\} = \left\{ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \right\}$$

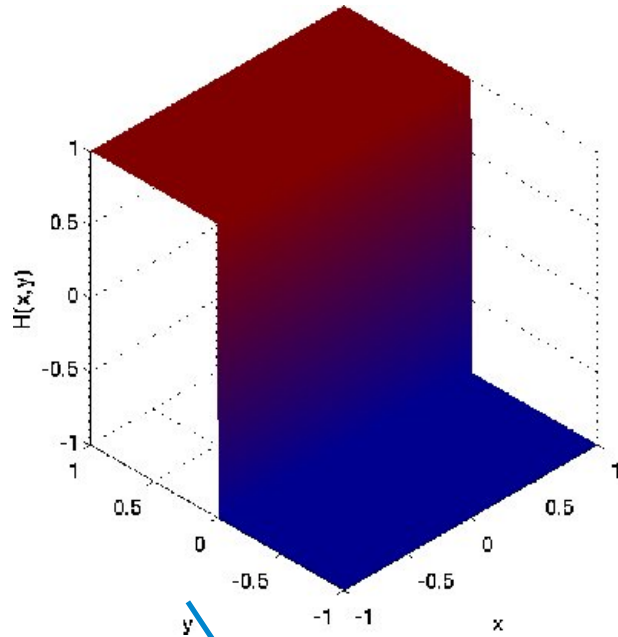
Enriched nodes

- - "Heaviside"
- - "crack tip"

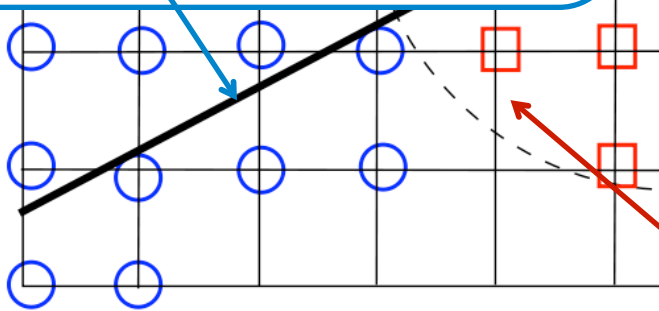
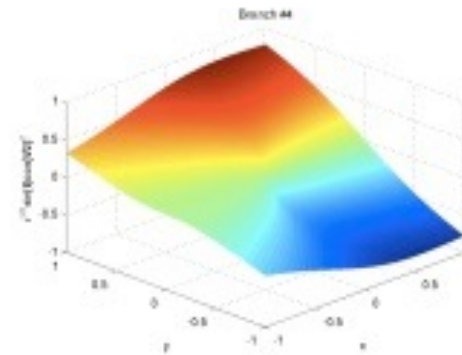
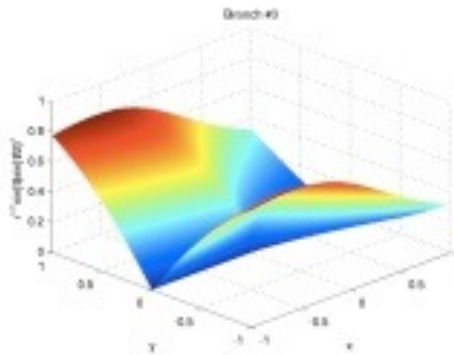
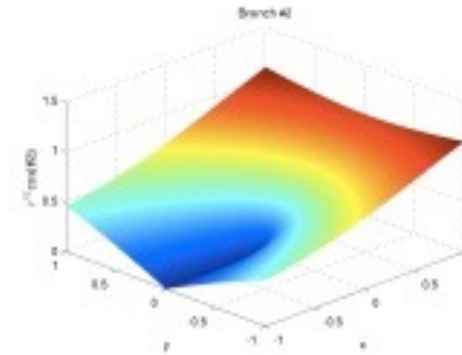
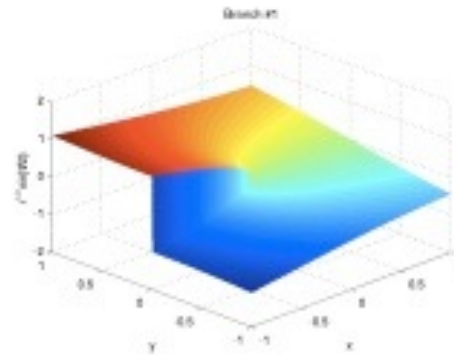


XFEM formulation

$$H(x) = \begin{cases} +1 & \text{if } x \text{ above crack} \\ -1 & \text{if } x \text{ below crack} \end{cases}$$



$$B(r, \theta) = \left\{ \sqrt{r} \cos \frac{\theta}{2} \quad \sqrt{r} \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \cos \frac{\theta}{2} \right\}$$



Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of “XFEM” using XFEM

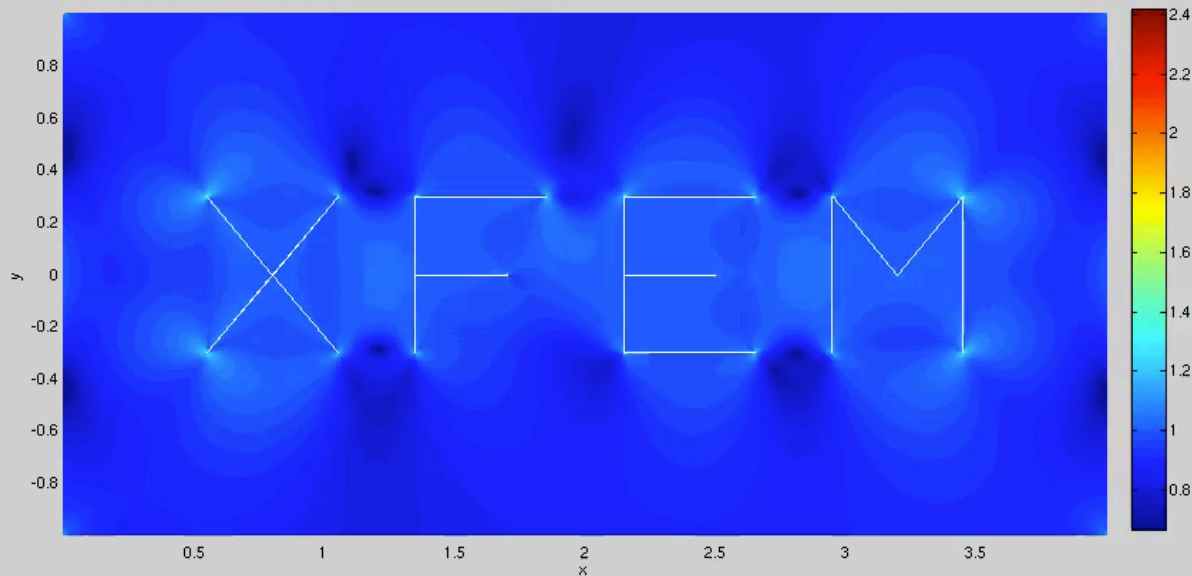
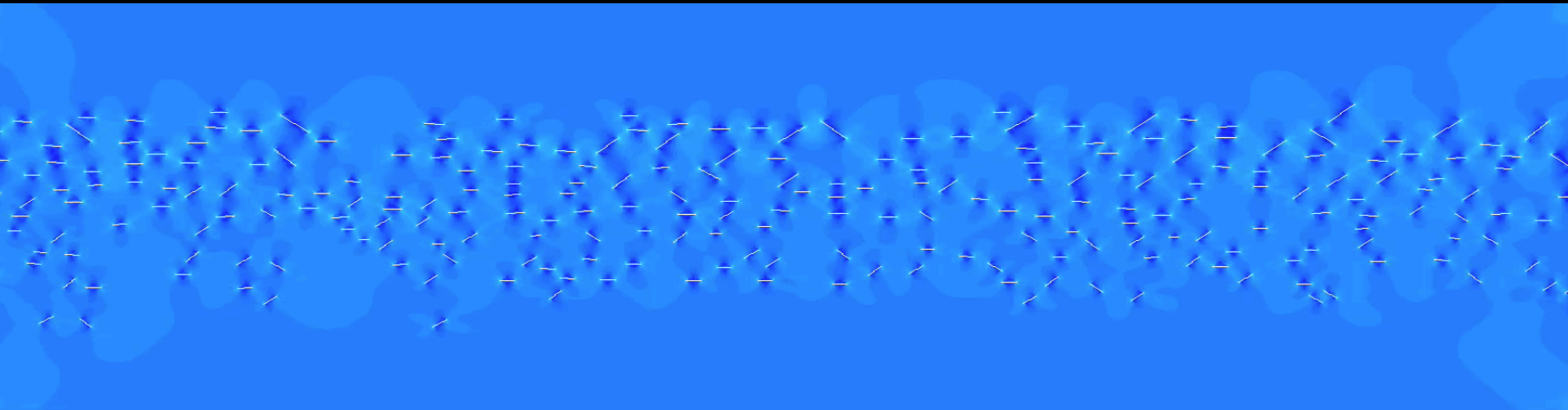
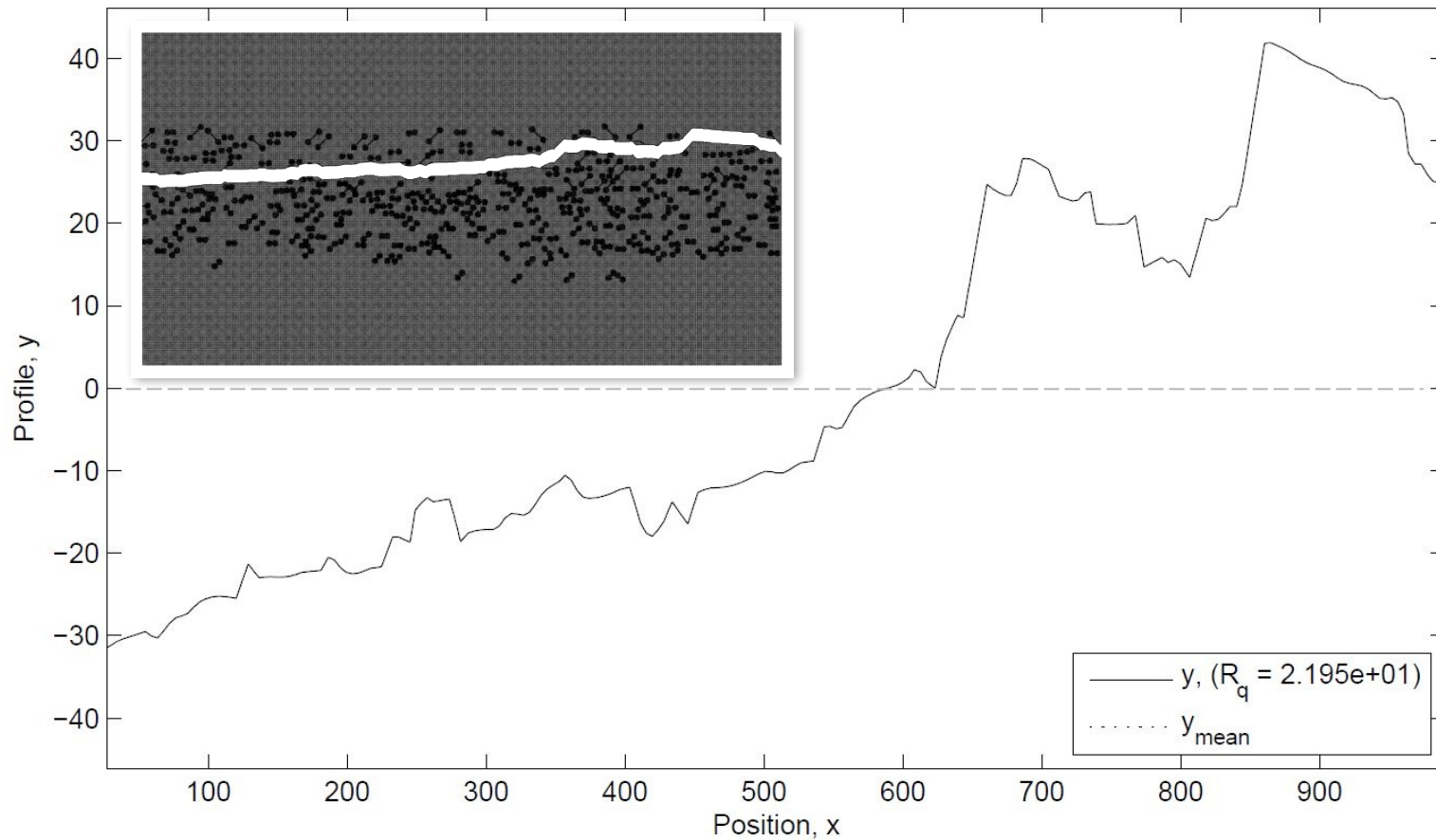


Plate with 300 cracks - vertical extension BCs



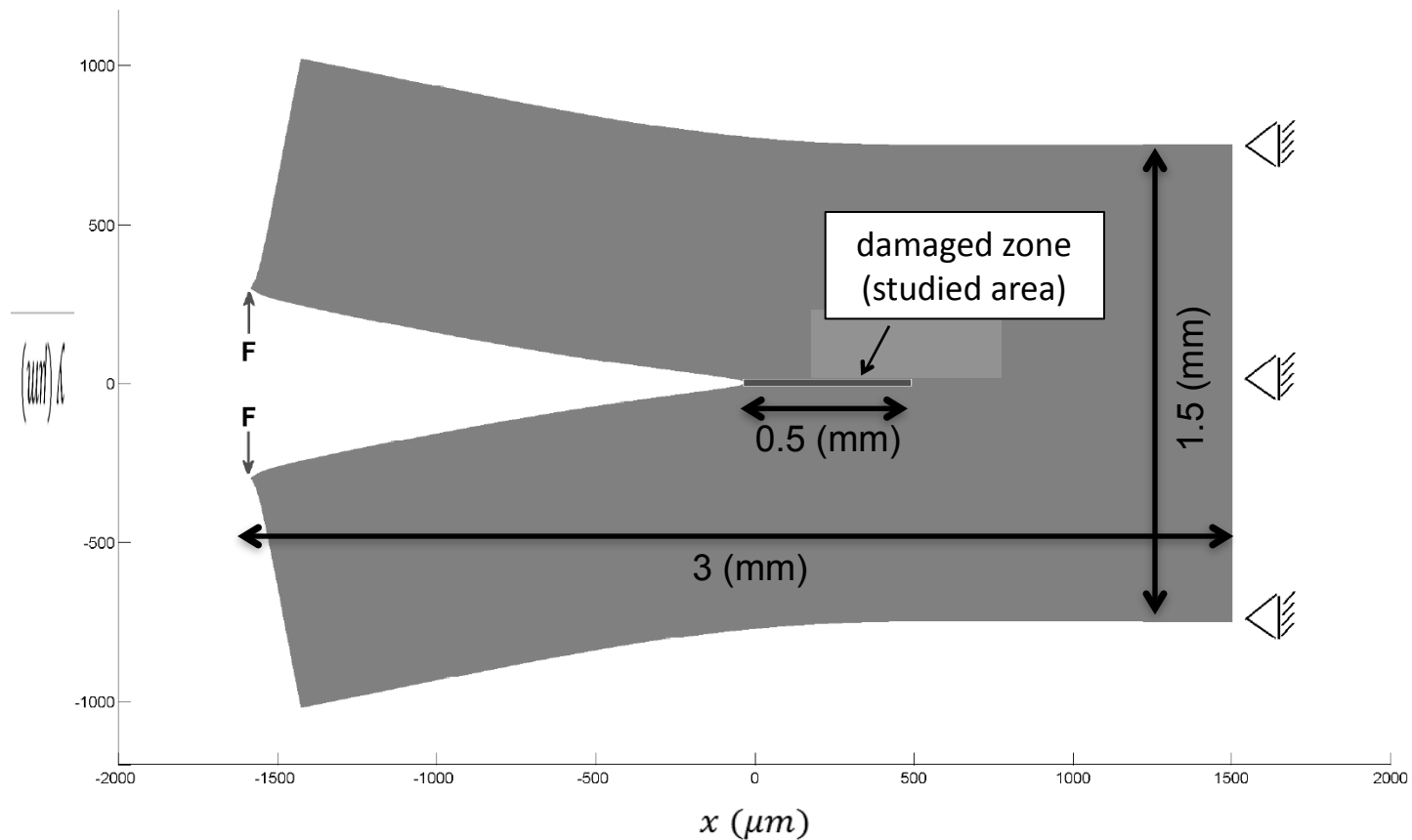
Vertical extension of a plate with 300 cracks

Post-split roughness



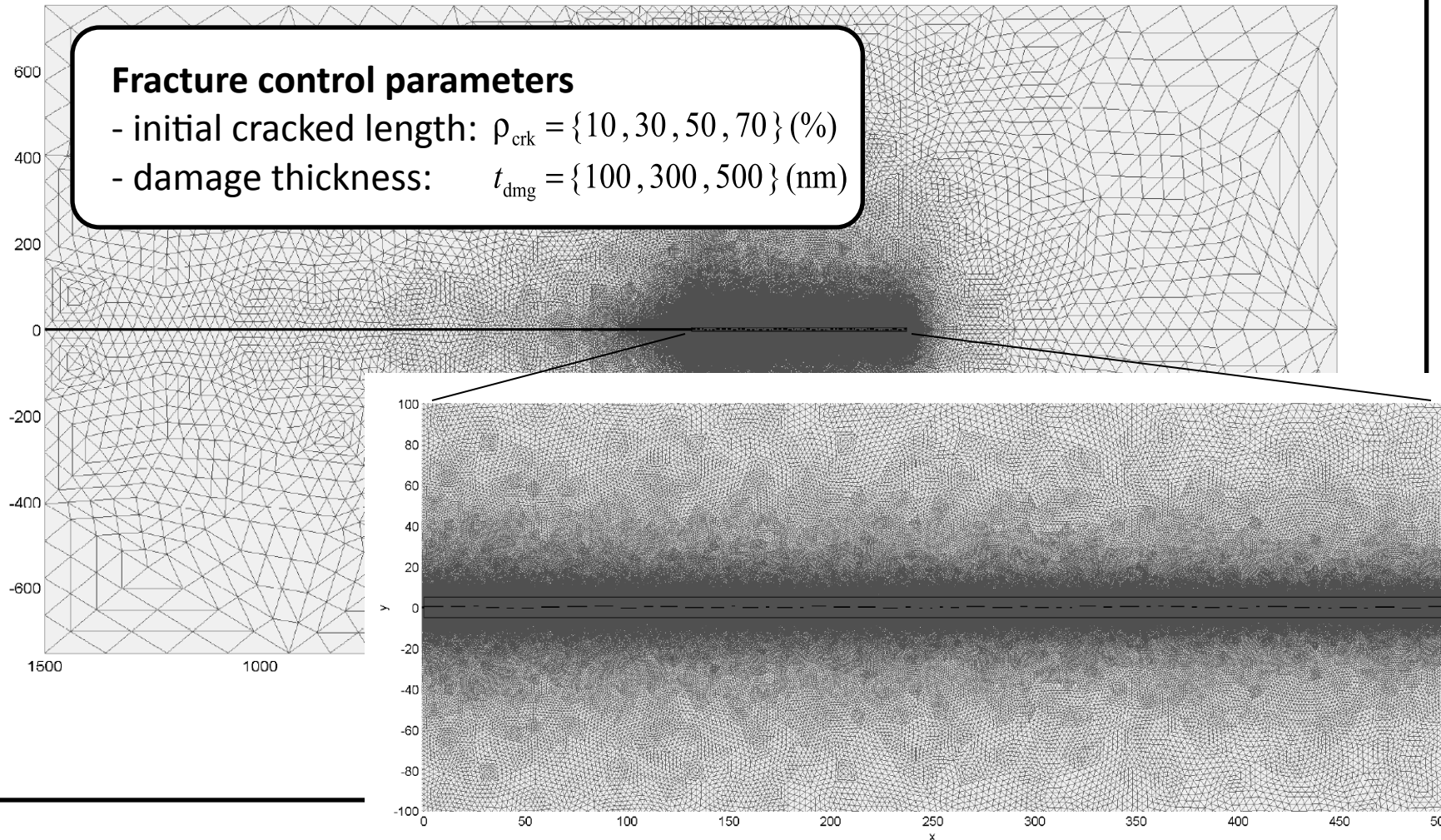
Mechanical splitting of a wafer sample

- Post-split roughness as a function of micro crack distribution



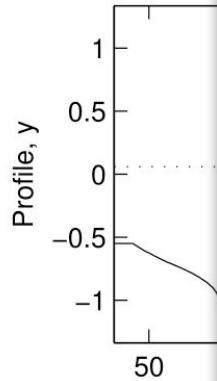
Mechanical splitting of a wafer sample

- Discretisation ($\approx 1\text{mln. DOF}$, $h_e = 150\text{ nm}$)

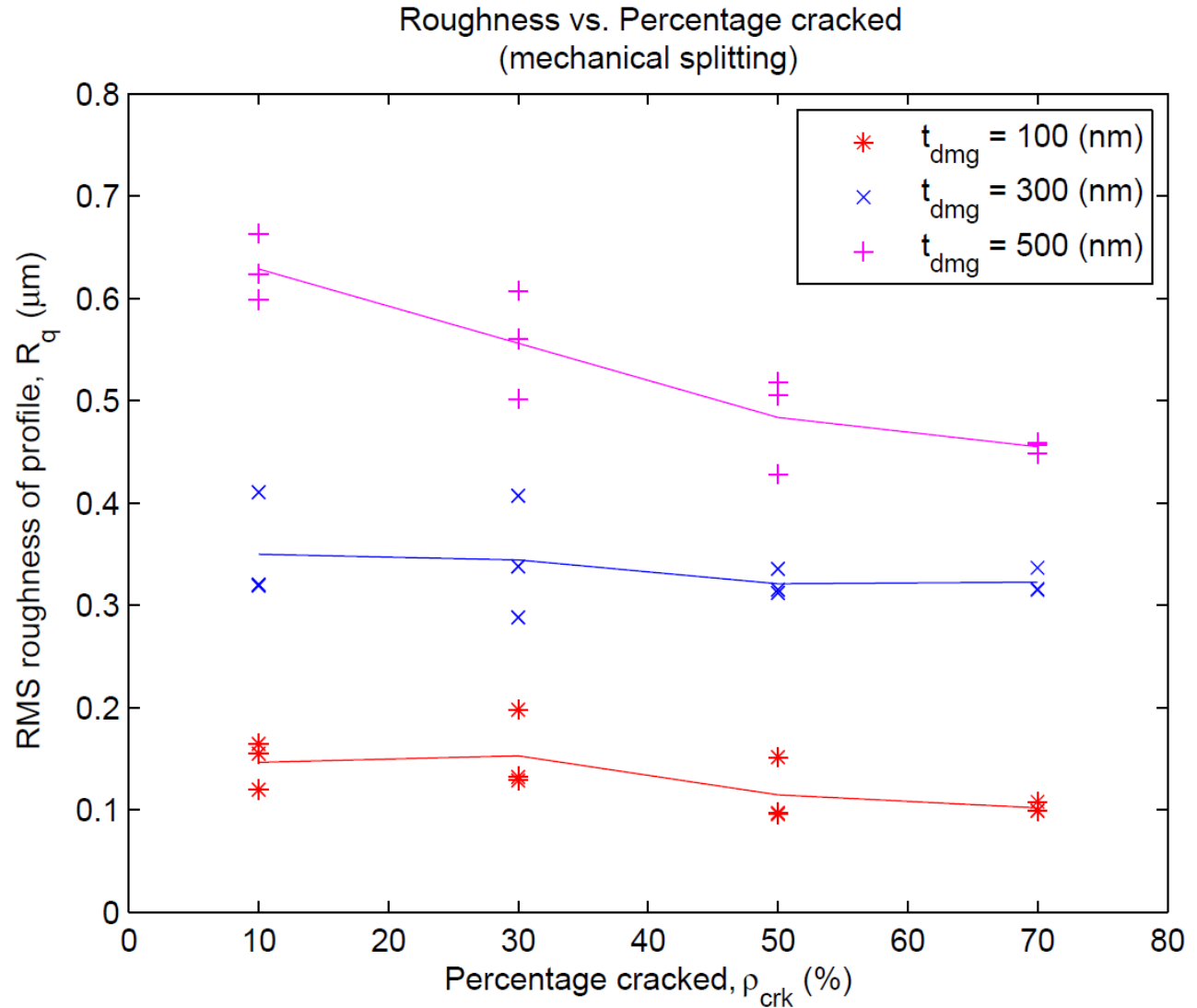
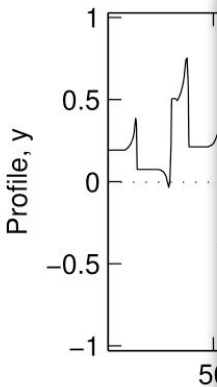


Fracture rou

- Case exar



- Case exar



Crack growth: classical approach (LEFM)

Evaluation of stress intensity factors (SIF)

- The interaction integral (Yau 1980)

(1) – from current solution
(2) – known auxiliary solution

$$I^{(1+2)} = \int_{\Omega} \left(\sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} + \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} - W^{(1+2)} \delta_{1j} \right) \frac{\partial q}{\partial x_j} d\Omega = \frac{2}{E'} (K_I^{(1)} K_I^{(2)} + K_{II}^{(1)} K_{II}^{(2)})$$

Crack growth criterion for mixed mode fracture

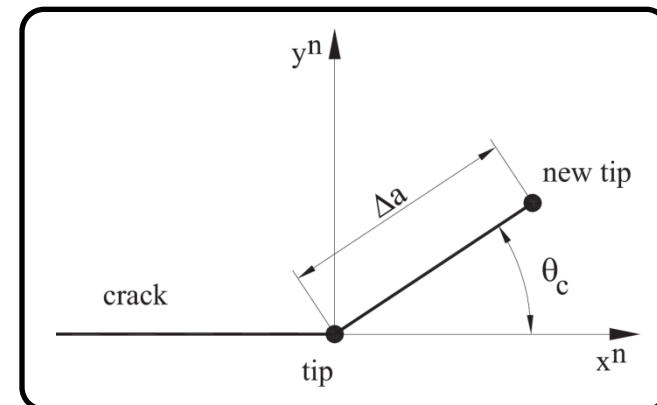
- Direction that maximises the energy release (Nuismer 1975)

$$\frac{k_I^2(K_I, K_{II}, \theta_{\text{inc}}) + k_{II}^2(K_I, K_{II}, \theta_{\text{inc}})}{E'} = G_c$$

Crack growth direction

- orthogonal to maximum hoop stress

$$\theta_c(K_I, K_{II}) = 2 \tan^{-1} \left[\frac{1}{4} \left(\frac{K_I}{K_{II}} - \text{sign}(K_{II}) \sqrt{\left(\frac{K_I}{K_{II}} \right)^2 + 8} \right) \right]$$



Crack growth: classical approach (LEFM)

- **Energy release rate w.r.t crack increment direction:**

$$G s_i = - \frac{\partial \Pi}{\partial \theta_i}$$

- **The rates of the energy release rate are given by:**

$$H s_{i,j} = \frac{\partial G s_i}{\partial \theta_j} = - \frac{\partial^2 \Pi}{\partial \theta_i \partial \theta_j}$$

- **where, in a discrete setting, the potential energy is:**

$$\Pi = \frac{1}{2} u' K u - u' f$$

Crack growth: optimization of direction

- **The discrete potential energy:**

$$\Pi = \frac{1}{2}u'Ku - u'f$$

- **The discrete energy release rate:**

$$Gs_i = -\frac{1}{2}u'\delta_i Ku + u'\delta_i f - \delta_i u'(Ku - f)$$

$$Gs_i = -\frac{1}{2}u'\delta_i Ku + u'\delta_i f \quad , \text{ where } \delta_i = \frac{\partial}{\partial \theta_i}$$

- **The rates of the energy release rate**

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ij}^2 Ku - u'\delta_{ij}^2 f\right) - \delta_j u'(\delta_i Ku - \delta_i f) \quad , \text{ where } \delta_{ij} = \frac{\partial^2}{\partial \theta_i \partial \theta_j}$$

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ii}^2 Ku - u'\delta_{ii}^2 f\right) + (\delta_j Ku - \delta_j f)'K^{-1}(\delta_i Ku - \delta_i f)$$

Crack growth: optimization of direction

- The discrete potential energy:

$$\Pi = \frac{1}{2}u'Ku - u'f$$

- The discrete energy release rate:

$$Gs_i = -\frac{1}{2}u'\delta_i Ku + u'\delta_i f - \delta_i u'(Ku - f)$$

$$Gs_i = -\frac{1}{2}u'\delta_i Ku + u'\delta_i f$$

- The rates of the energy release rate

$$\delta u = -K^{-1}(\delta Ku - \delta f)$$

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ij}^2 Ku - u'\delta_{ij}^2 f\right) - \delta_j u'(\delta_i Ku - \delta_i f)$$

expensive

$$Hs_{ij} = -\left(\frac{1}{2}u'\delta_{ii}^2 Ku - u'\delta_{ii}^2 f\right) + (\delta_j Ku - \delta_j f)' K^{-1}(\delta_i Ku - \delta_i f)$$

remote interaction

Crack growth: optimization of direction

$$\delta \mathbf{K}_e = \int_{\Omega_e} (\delta \mathbf{B}^T \mathbf{D} \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta \mathbf{B}) \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} \mathbf{B}^T \mathbf{D} \mathbf{B} \delta \det(\mathbf{J}) d\bar{\Omega}$$

$$\delta^2 \mathbf{K}_e = \int_{\Omega_e} (\delta^2 \mathbf{B}^T \mathbf{D} \mathbf{B} + 2\delta \mathbf{B}^T \mathbf{D} \delta \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta^2 \mathbf{B}) \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} 2(\delta \mathbf{B}^T \mathbf{D} \mathbf{B} + \mathbf{B}^T \mathbf{D} \delta \mathbf{B}) \delta \det(\mathbf{J}) d\bar{\Omega} + \int_{\Omega_e} \mathbf{B}^T \mathbf{D} \mathbf{B} \delta^2 \det(\mathbf{J}) d\bar{\Omega}$$

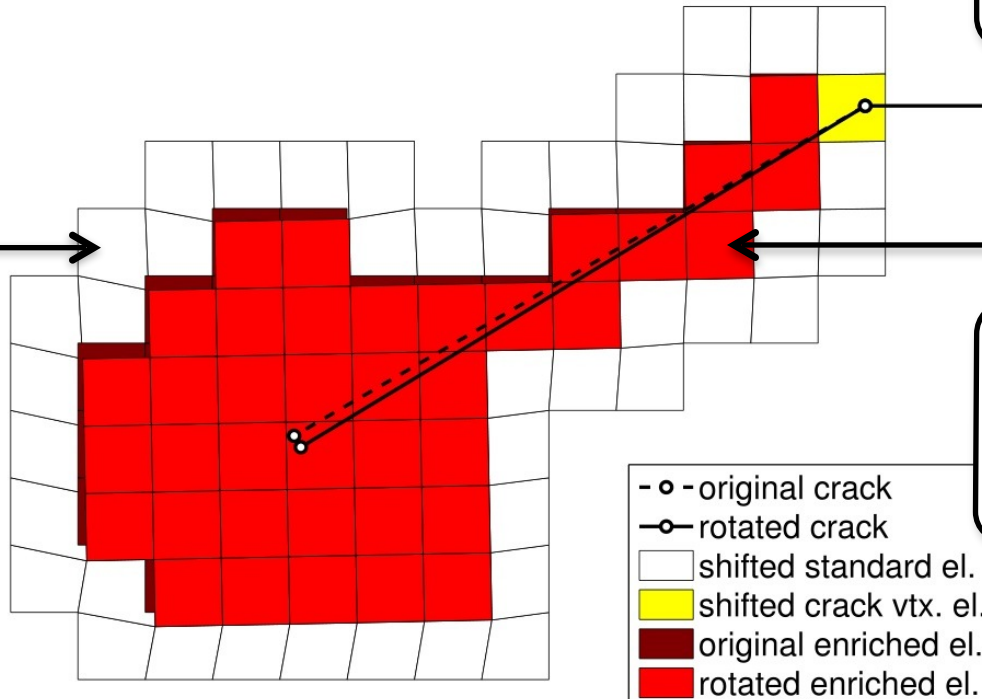
Differentiation of the stiffness matrix
w.r.t. crack increment direction

$$\delta \mathbf{K}_e = \mathbf{T}^T \mathbf{K}_e + \mathbf{K}_e \mathbf{T}$$

$$\delta^2 \mathbf{K}_e = 2(\mathbf{T}^T \mathbf{K}_e \mathbf{T} - \mathbf{K}_e)$$

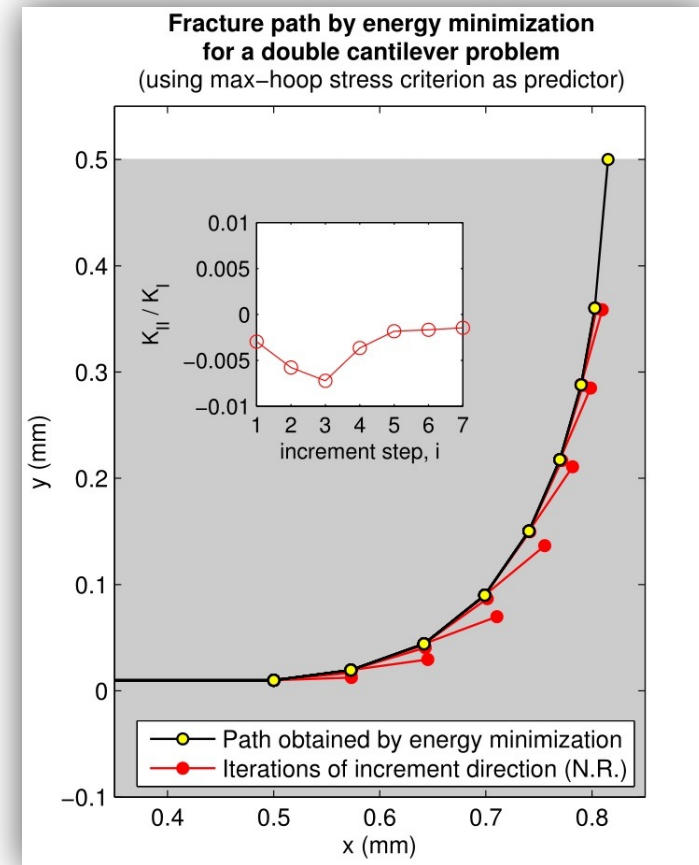
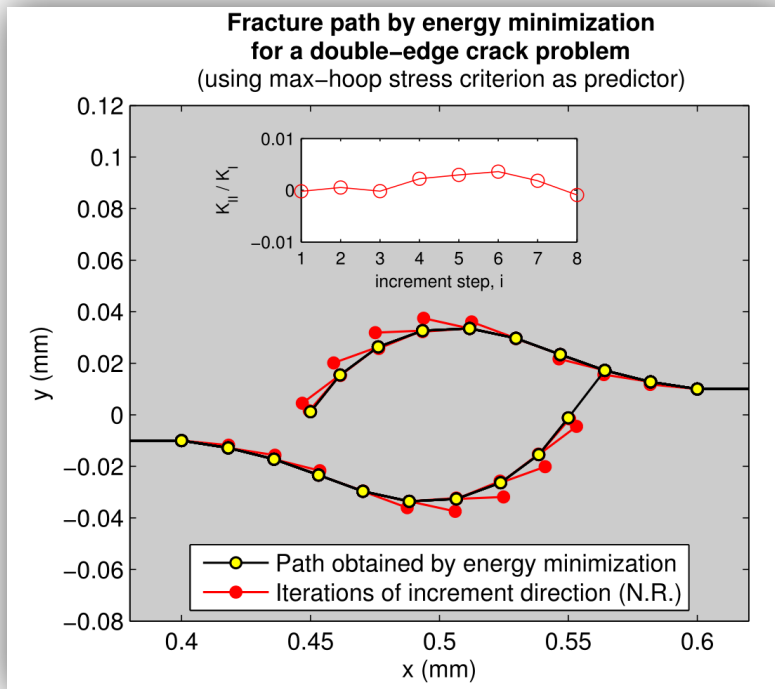
Updated directions:

$$\theta^{k+1} = \theta^k - \mathbf{H}_s^{-1} \mathbf{G}_s$$



Crack growth: optimization of direction

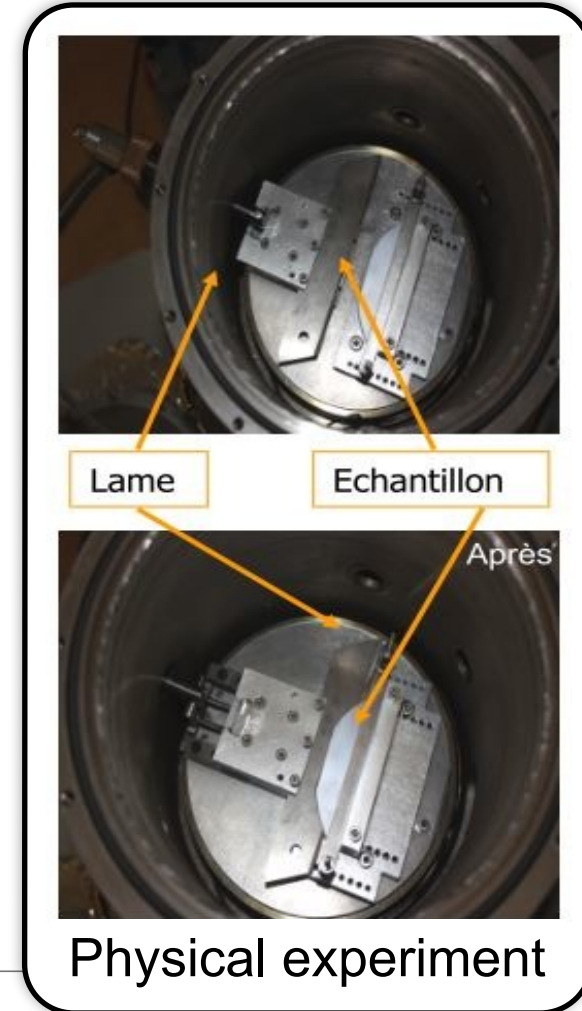
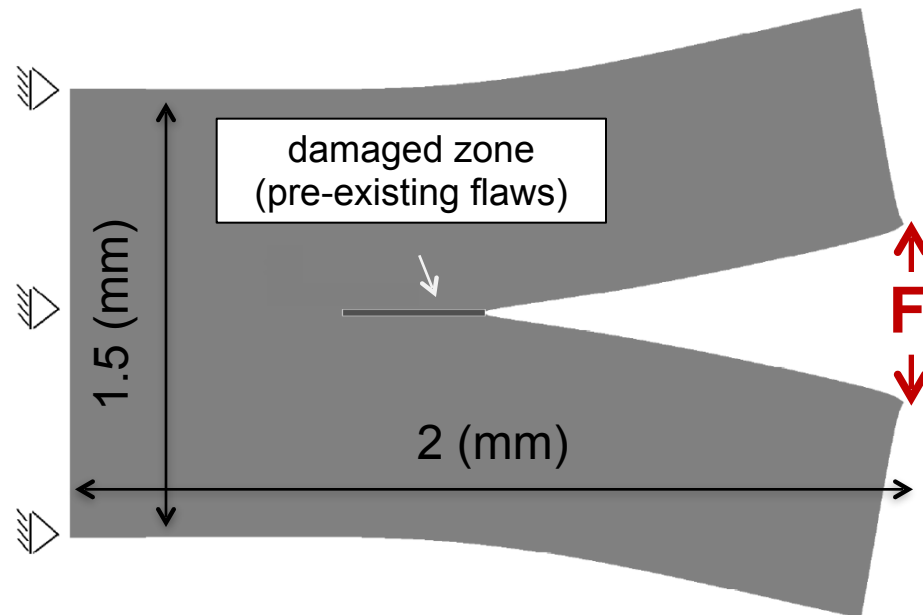
- **Energy minimization w.r.t. to a finite crack propagation**
 - The growth direction is given by satisfying: $\partial\Pi/\partial\theta_i = 0$
 - Using the maximum hoop-stress criterion as initial guess
- **Numerical examples:**



Application to Si-wafer splitting

Mechanical splitting of a wafer

- Post-split roughness as a function of micro crack distribution
- Consider a representative material sample
- BC: blade loading = fixed displacements (RHS)
- 20 initial micro cracks within the damage zone



Application to Si-wafer splitting

Mechanical splitting of a wafer

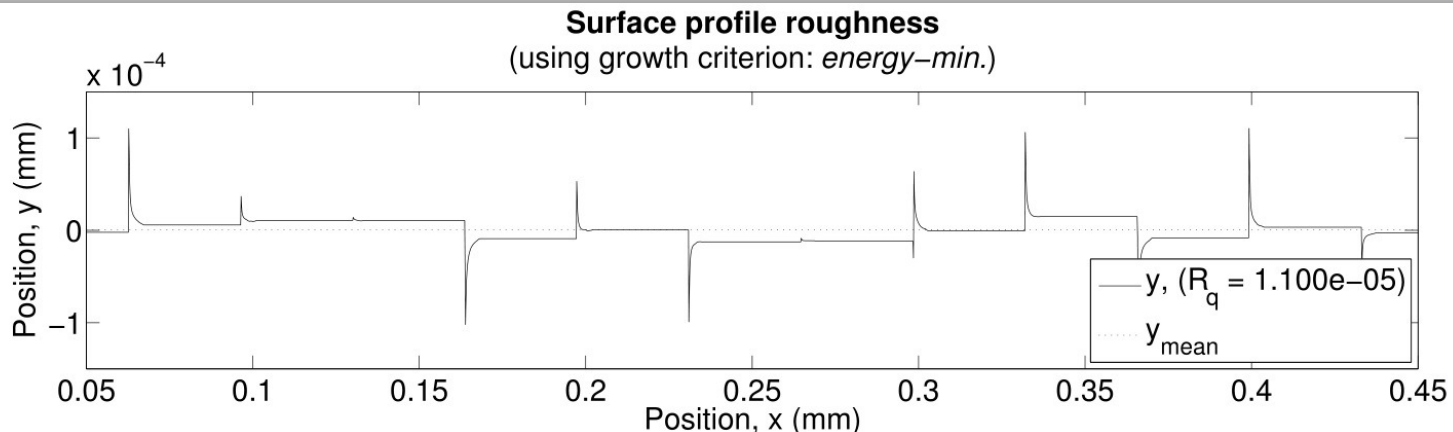
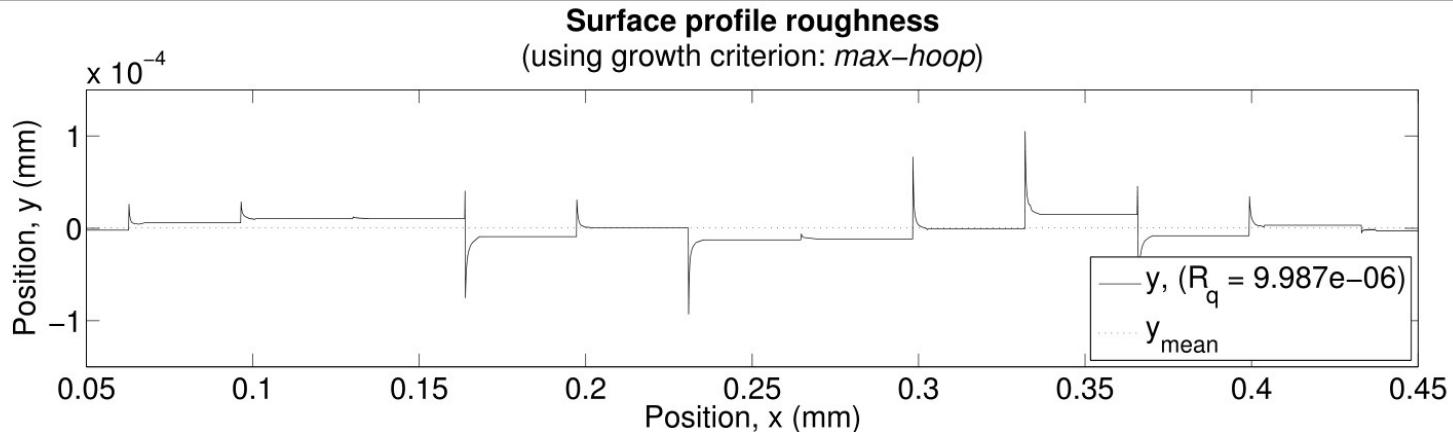
- Fracture path comparison: *max-hoop crit.* VS. *energy min.*
- NOTE: non-uniform scaling of axis, $y / x = 400$

Si-wafer splitting using a wedge blade
(comparison of two growth criteria)

Application to Si-wafer splitting

Mechanical splitting of a wafer

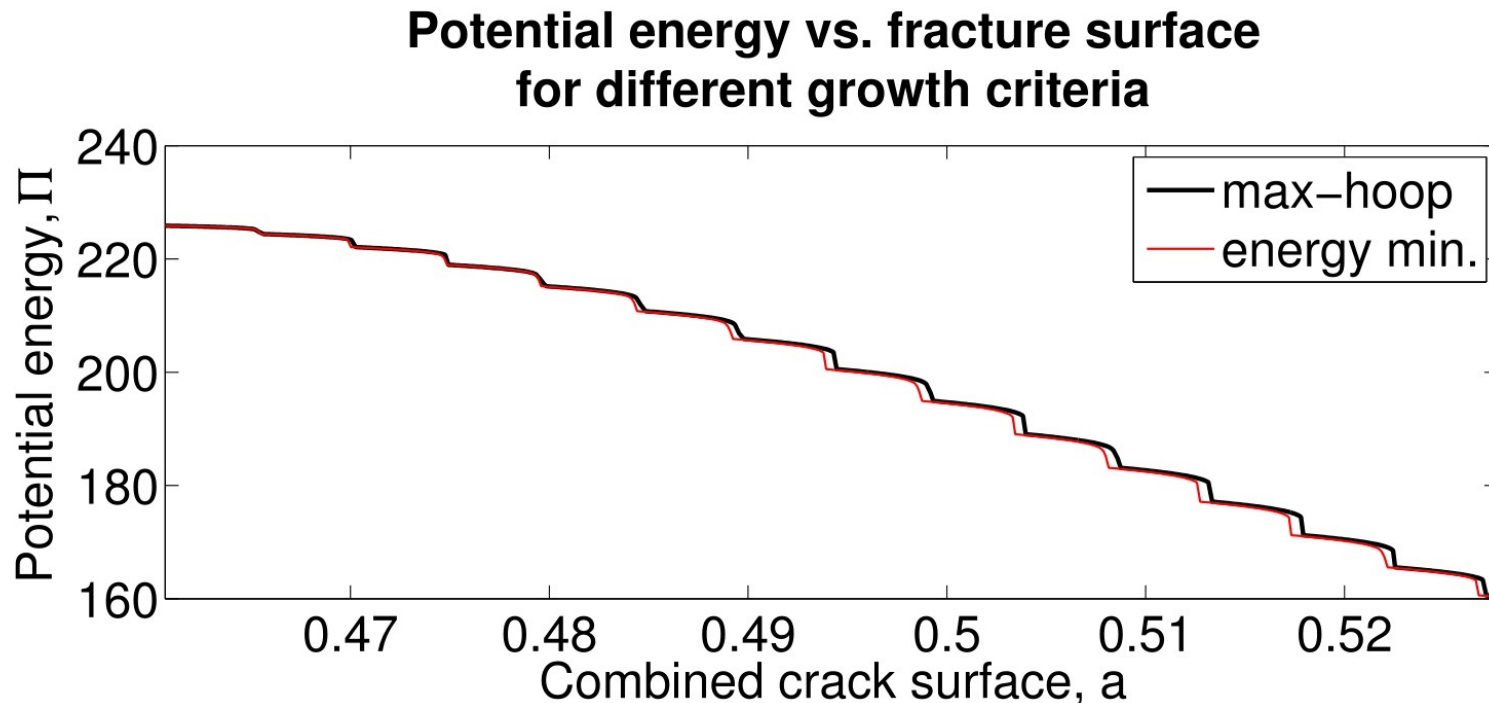
- Comparison of post-split fracture surface roughness



Application to Si-wafer splitting

Mechanical splitting of a wafer

- Comparison of total (potential) energy



Part IV. Application to surgical simulation

with Institut of Advanced Studies (iCube, University of Strasbourg, France: Hadrien Courtecuisse), INRIA, SHACRA Team (Stéphane Cotin, Christian Duriez); Karol Miller, UWA.

Faculty of Sciences,
Technology
and Communication

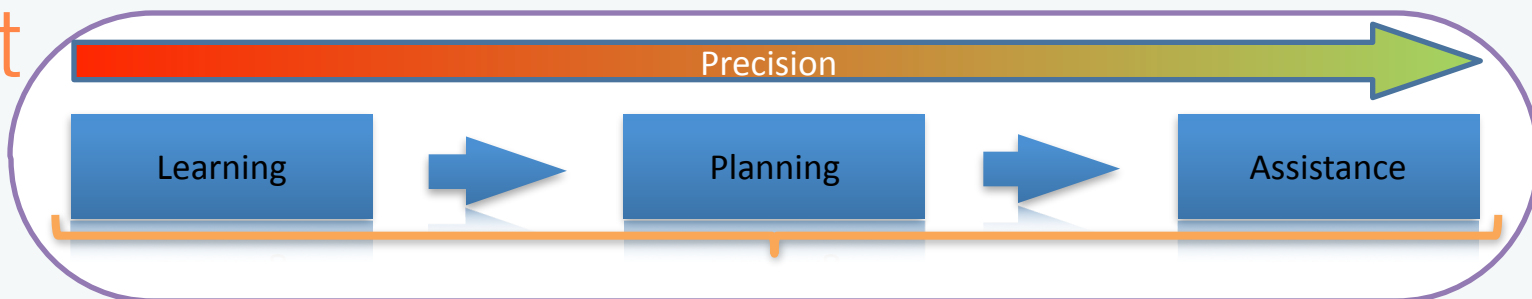


RealTcut

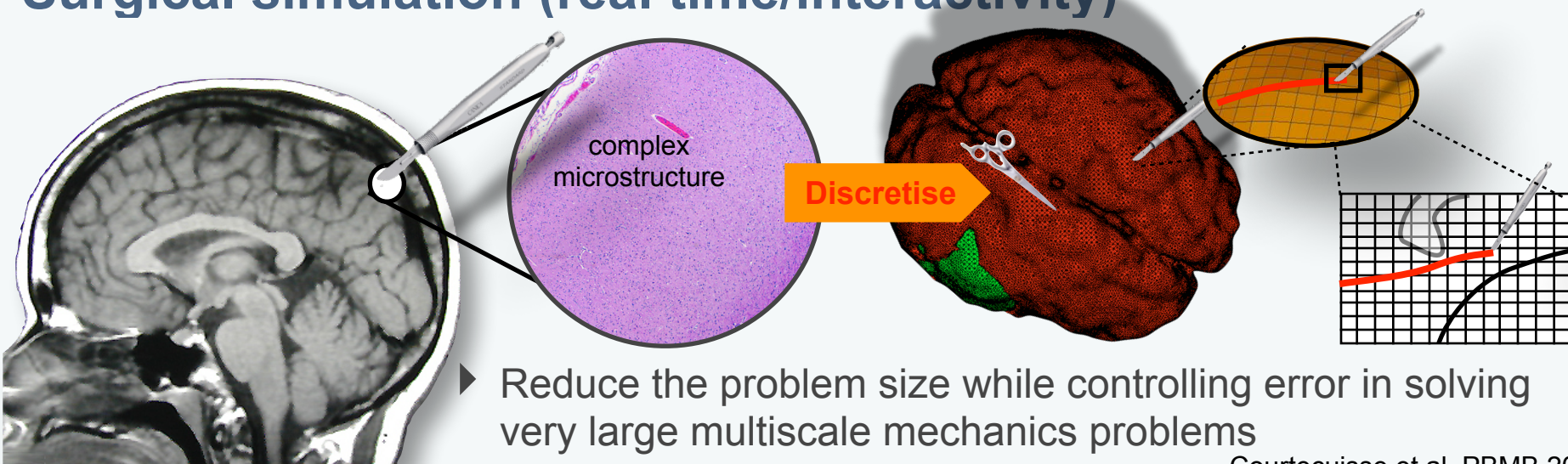
Interactive multiscale
cutting simulations



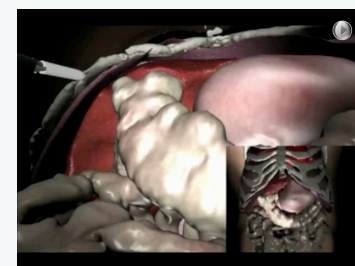
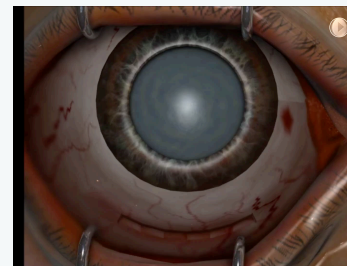
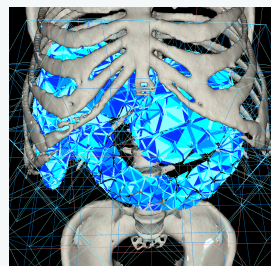
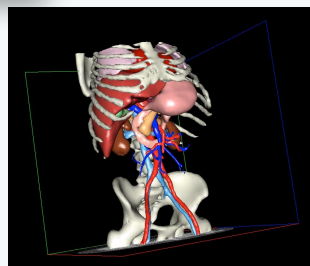
RealTcut



Surgical simulation (real time/interactivity)



Courtecuisse et al. PBMB 2011



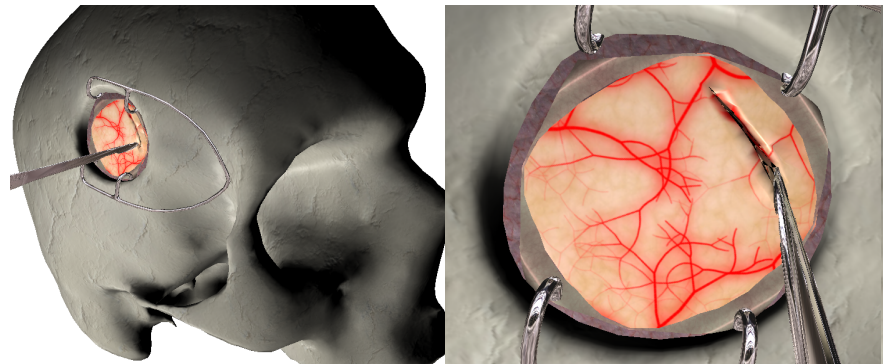
Concrete objective: compute the response of organs during surgical procedures (including cuts) in real time (50-500 solutions per second)

Two schools of thought

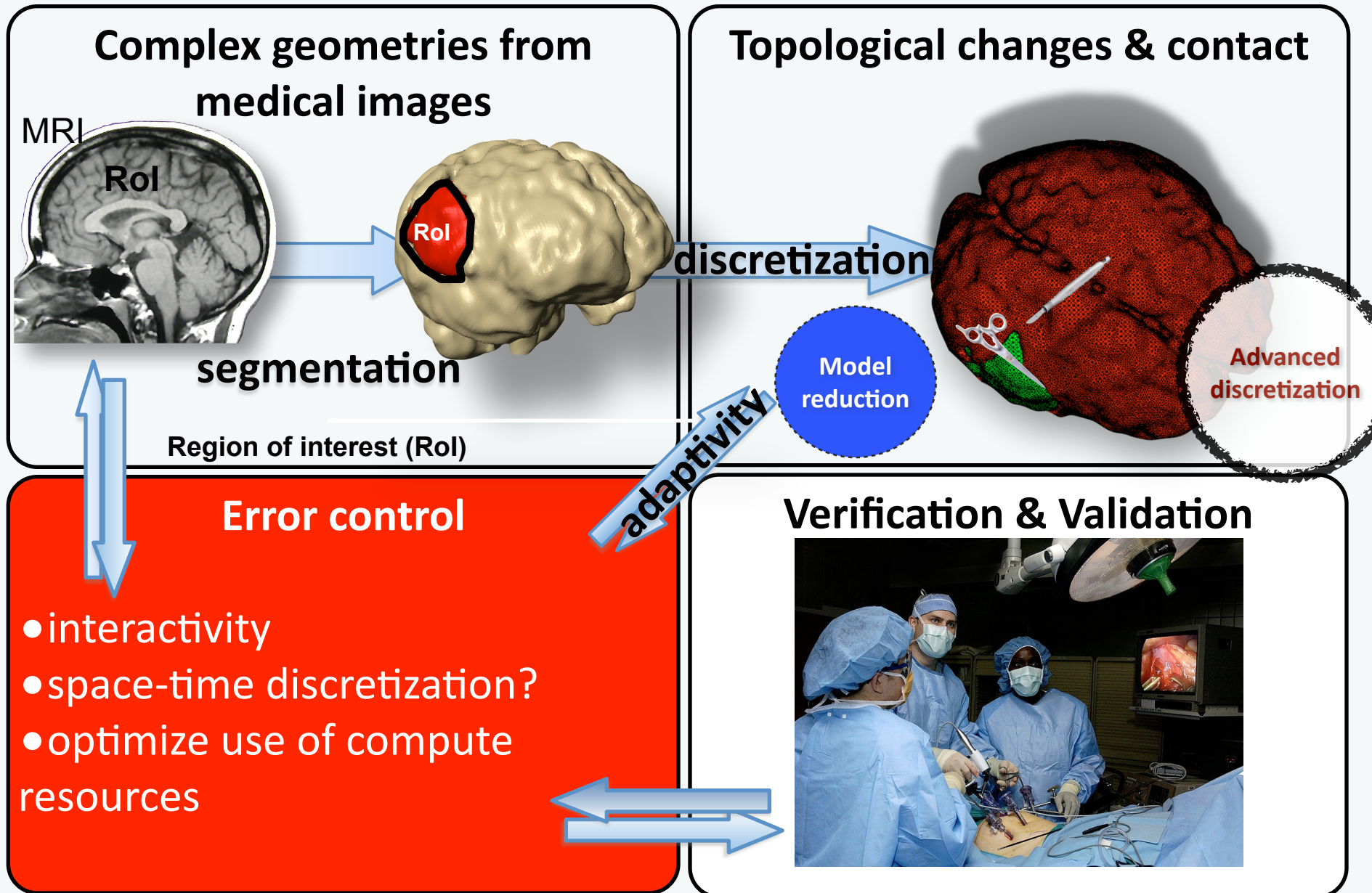
- ▶ constant time
 - ➡ accuracy often controlled visually only
- ▶ model reduction or “learning”
 - ➡ scarce development for biomedical problems
 - ➡ no results available for cutting

Proposed approach: maximize accuracy for given computational time. Error control

First implicit, interactive method for cutting with contact

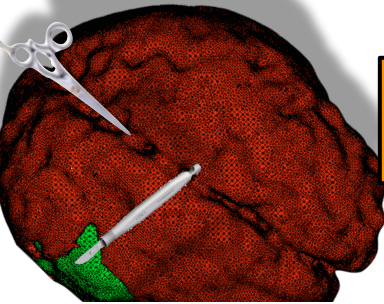


[Courtecuisse et al., MICCAI, 2013]
Collaboration INRIA



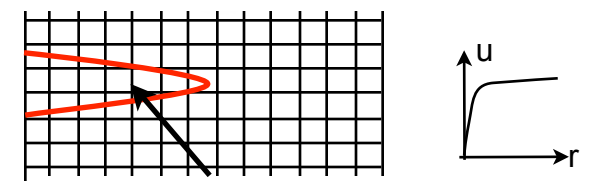
calculs **offline**

génération solutions particulières



$\sim 10^6$
snapshots

calcul champs asymptotiques



action de l'instrument

tri
pré-opératoire

$\sim 10^3$
snapshots

"mapping"
spécifique
patient

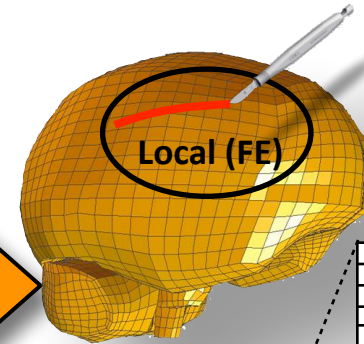
enrichissement "pointe
de coupe"

POD

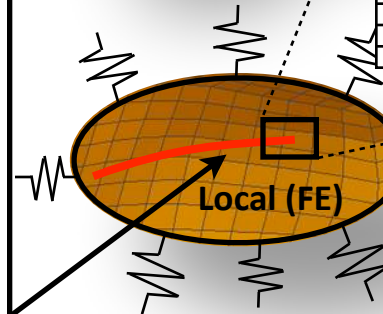
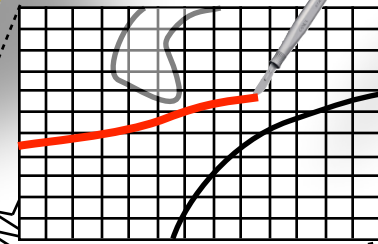
$O(10)$ fonctions

espace
réduit de
petite
dimension

calculs **online**: interactivité



représentation
locale



approximation
POD globale



A semi-implicit method for real-time deformation, topological changes, and contact of soft tissues

Paper ID : 269

EPSRC

Pioneering research
and skills

THE ROYAL
SOCIETY

hpc
CYMRU WALES

SEVENTH FRAMEWORK
PROGRAMME

Acknowledgements

The Leverhulme Trust

The Royal Academy
of Engineering

INRIA
INVENTEURS DU MONDE NUMÉRIQUE

European Research Council

erc

IDEAS

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PERMIX: Multiscale, XFEM, large deformation, coupled 2 LAMMPS, ABAQUS, OpenMP -
Fortran 2003, C++

MATLAB Codes: XFEM, 3D ISOGEOMETRIC XFEM, 2D ISOGEOMETRIC BEM, 2D MESHLESS
DOWNLOAD @ <http://cmechanicsos.users.sourceforge.net/>

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the group...
November 2012



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thank you



Yusuf Ghaffari
Stagh

Andrés Octavio
Estrada

Chi Hoang



Hadrien
Courtecuisse



Olivier
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Daniel Paladim



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Lee



Dr. Robert Simpson



Dr. Pierre Kerfriden

Publications - model reduction

- <http://orbilu.uni.lu/handle/10993/12024>
- <http://orbilu.uni.lu/handle/10993/12012>
- <http://orbilu.uni.lu/handle/10993/10207>
- <http://orbilu.uni.lu/handle/10993/12454>
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Mesh-burden reduction

- <http://orbilu.uni.lu/handle/10993/12159>
- <http://orbilu.uni.lu/handle/10993/14135>
- <http://orbilu.uni.lu/handle/10993/13847>
- <http://orbilu.uni.lu/handle/10993/12157>
- <http://orbilu.uni.lu/handle/10993/11850>

Demos

- Surgical simulation
 - <http://www.youtube.com/watch?v=KqM7rh6sE8s>
 - <http://www.youtube.com/watch?v=DYBRKbEiHj8>
- Multi-crack growth
 - <http://www.youtube.com/watch?v=6yPb6NXnex8>
 - <http://www.youtube.com/watch?v=7U2o5bFvj8E>

Demos

- <http://www.youtube.com/watch?v=90NAq76mVmQ>
- Solder joint durability
 - <http://www.youtube.com/watch?v=Ri96Wv6zBNU>
 - http://www.youtube.com/watch?v=1g3Pe_9XN9I

Damage tolerance assessment directly from CAD

- <http://www.youtube.com/watch?v=RV0gidOT0-U>
- <http://www.youtube.com/watch?v=cYhaj6SPLTE>
- <http://orbilu.uni.lu/handle/10993/12159>
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- <http://orbilu.uni.lu/handle/10993/13847>
- <http://orbilu.uni.lu/handle/10993/12157>

Damage tolerance analysis directly from CAD

- <http://orbilu.uni.lu/handle/10993/11850>



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- T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. CMAME, 194(39-41):4135–4195, 2005.
- J. A. Cottrell, T. J.R. Hughes, and Y. Bazilevs. Isogeometric Analysis: Toward Integration of CAD and FEA. Wiley, 2009.



- P. Kagan, A. Fischer, and P. Z. Bar-Yoseph. New B-Spline Finite Element approach for geometrical design and mechanical analysis. *IJNME*, 41(3):435–458, 1998.
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- **T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *CMAME*, 194(39-41):4135–4195, 2005.**
- J. A. Cottrell, T. J.R. Hughes, and Y. Bazilevs. *Isogeometric Analysis: Toward Integration of CAD and FEA*. Wiley, 2009.



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MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg Computer Methods in Applied Mechanics and Engineering, 2013.



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- <http://orbilu.uni.lu/handle/10993/12454>
- <http://orbilu.uni.lu/handle/10993/12453>
- <http://orbilu.uni.lu/handle/10993/14475>
- <http://orbilu.uni.lu/handle/10993/10206>

Mesh-burden reduction

- <http://orbilu.uni.lu/handle/10993/12159>
- <http://orbilu.uni.lu/handle/10993/14135>
- <http://orbilu.uni.lu/handle/10993/13847>
- <http://orbilu.uni.lu/handle/10993/12157>
- <http://orbilu.uni.lu/handle/10993/11850>

Demos

- Surgical simulation
 - <http://www.youtube.com/watch?v=KqM7rh6sE8s>
 - <http://www.youtube.com/watch?v=DYBRKbEiHj8>
- Multi-crack growth
 - <http://www.youtube.com/watch?v=6yPb6NXnex8>
 - <http://www.youtube.com/watch?v=7U2o5bFvj8E>

Demos

- <http://www.youtube.com/watch?v=90NAq76mVmQ>
- Solder joint durability
 - <http://www.youtube.com/watch?v=Ri96Wv6zBNU>
 - http://www.youtube.com/watch?v=1g3Pe_9XN9I

Damage tolerance assessment directly from CAD

- <http://www.youtube.com/watch?v=RV0gidOT0-U>
- <http://www.youtube.com/watch?v=cYhaj6SPLTE>
- <http://orbilu.uni.lu/handle/10993/12159>
- <http://orbilu.uni.lu/handle/10993/14135>
- <http://orbilu.uni.lu/handle/10993/13847>
- <http://orbilu.uni.lu/handle/10993/12157>

Damage tolerance analysis directly from CAD

- <http://orbilu.uni.lu/handle/10993/11850>